R for Photobiology

A handbook

Pedro J. Aphalo,
Andreas Albert
and
Titta Kotilainen

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Preface

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

Acknowledgements

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List of abbreviations and symbols

For quantities and units used in photobiology we follow, as much as possible, the recommendations of the Commission Internationale de l'Éclairage as described by (Sliney 2007).

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

E_0	fluence rate, also called scalar irradiance ($\mathrm{W\,m^{-2}}$).
ESR	early stage researcher.
FACE	free air carbon-dioxide enhancement.
FEL	a certain type of 1000 W incandescent lamp.
FLAV	UV action spectrum for accumulation of flavonoids.
FWHM	full-width half-maximum.
GAW	Global Atmosphere Watch.
GEN	generalized plant action spectrum, also abreviated as GPAS (Caldwell 1971).
GEN(G)	mathematical formulation of GEN by (Green et al. 1974) .
GEN(T)	mathematical formulation of GEN by (Thimijan et al. 1978).
h	Planck's constant.
h'	Planck's constant per mole of photons.
H	exposure, frequently called dose by biologists ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
H^{BE}	biologically effective (energy) exposure ($\mathrm{kJ\,m^{-2}\,d^{-1}}$).
$H_{\mathrm{p}}^{\mathrm{BE}}$	biologically effective photon exposure ($\mathrm{mol\,m^{-2}\,d^{-1}}$).
HPS	high pressure sodium, a type of discharge lamp.
HSD	honestly signifcant difference.
k_{B}	Boltzmann constant.
L	radiance ($\mathrm{W\,sr^{-1}\,m^{-2}}$).
LAI	leaf area index, the ratio of projected leaf area to the ground area.
LED	light emitting diode.
LME	linear mixed effects (type of statistical model).
LSD	least significant difference.
n	number of replicates (number of experimental units per treatment).
N	total number of experimental units in an experiment.
N_{A}	Avogadro constant (also called Avogadro's number).
NIST	National Institute of Standards and Technology (U.S.A.).
NLME	non-linear mixed effects (statistical model).
OTC	open-top chamber.
PAR	, 400–700 nm.
	measured as energy or photon irradiance.
PC	polycarbonate, a plastic.
PG	UV action spectrum for plant growth.
PHIN	UV action spectrum for photoinhibition of isolated chloroplasts.
PID	(control algorithm).
PMMA	polymethylmethacrylate.
PPFD	, another name for
	PAR photon irradiance (Q_{PAR}).
PTFE	polytetrafluoroethylene.
PVC	polyvinylchloride.
q	energy in one photon ('energy of light').
q'	energy in one mole of photons.
Q	photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}}$).
$Q(\lambda)$	spectral photon irradiance ($\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$ or $\mathrm{\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}}$).
r_0	distance from sun to earth.
RAF	(nondimensional).
RH	relative humidity (%).
s	energy effectiveness (relative units).

$s(\lambda)$	spectral energy effectiveness (relative units).
s^{p}	quantum effectiveness (relative units).
$s^{\mathrm{p}}(\lambda)$	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 (λ = 100–400 nm).
UV-A	ultraviolet-A radiation (λ = 315–400 nm).
UV-B	ultraviolet-B radiation (λ = 280–315 nm).
UV-C	ultraviolet-C radiation (λ = 100–280 nm).
$\mathrm{UV}^{\mathrm{BE}}$	biologically effective UV radiation.
UTC	coordinated universal time, replaces GMT in technical use.
VIS	radiation visible to the human eye ($\approx$ 400–700 nm).
WMO	World Meteorological Organization.
VPD	water vapour pressure deficit (Pa).
WOUDC	World Ozone and Ultraviolet Radiation Data Centre.

Part I

Preliminaries

CHAPTER 1

Introduction

Abstract

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

1.1 Radiation and molecules

CHAPTER 2

Radiation physiscs

Abstract

In this chapter we explain how to .

2.1 Packages used in this chapter

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

```
library(photobiology)

## Loading required package:  data.table

library(photobiologygg)

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

library(photobiologyWavebands)
library(photobiologySun)
```

2.2 Ultraviolet and visible radiation

In a physical sense, ultraviolet (UV) and visible (VIS) radiation (i.e. also PAR) are 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

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

Table 2.1. The long wavelengths of solar radiation, called infrared (IR) radiation, are also listed. The colour ranges indicated in Table 2.1 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 (e.g. Aphalo, Albert, Björn, Ylianttila et al. 2012, Table xx)). 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,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \tag{2.1}$$

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 (2.1) 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

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \tag{2.2}$$

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 2.1 and 2.2 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 2.1 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, $d\Omega$, which is a two-dimensional angle in a space. The relation between dA and $d\Omega$ in spherical coordinates is geometrically explained in Figure 2.1.

[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 2.1.

Table 2.1: Regions of the electromagnetic radiation associated with colours, after (Iqbal 1983) and (Eichler et al. 1993) with alterations.

Colour	Wavelength (nm)	Frequency (THz)
UV-C	100 – 280	3000 – 1070
UV-B	280 – 315	1070 – 950
UV-A	315 – 400	950 – 750
violet	400 – 455	750 – 660
blue	455 – 492	660 – 610
green	492 – 577	610 – 520
yellow	577 – 597	520 – 502
orange	597 – 622	502 – 482
red	622 – 700	482 – 428
far red	700 – 770	428 – 390
near IR	770 – 3000	390 – 100
mid IR	3000 – 50000	100 – 6
far IR	50000 – 10^6	6 – 0.3

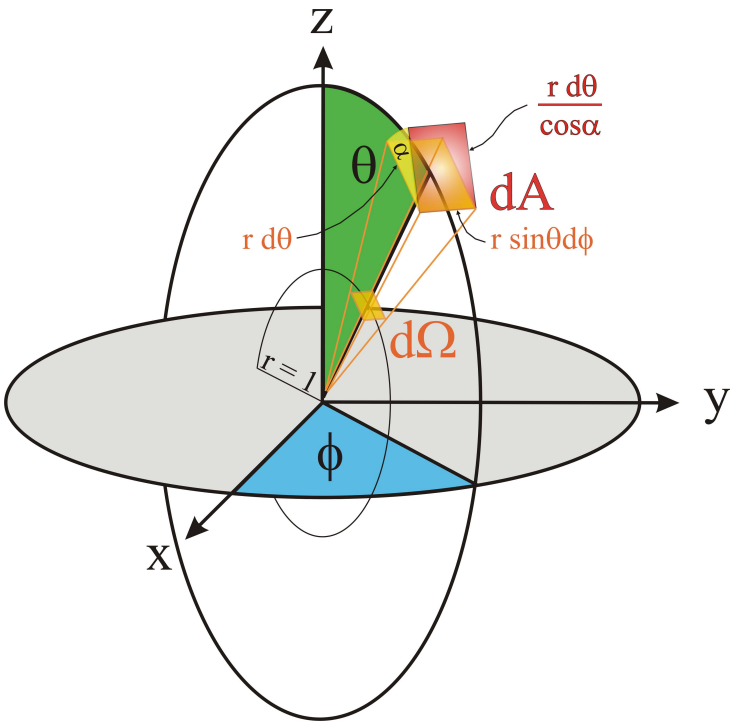


Figure 2.1: Definition of the solid angle dΩ and the geometry of areas in the space (redrawn after Eichler et al. 1993), where the given solid angle dΩ remains the same, regardless of distance r, while the exposed area exemplified by dA will change with distance r from the origin (light source) and the 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.

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

$$\mathrm{d}\Omega = \mathrm{d}\theta \cdot \sin\theta \mathrm{d}\phi \tag{2.3}$$

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:

$$\mathrm{d}A = \frac{r\mathrm{d}\theta}{\cos\alpha} \cdot r\sin\theta\mathrm{d}\phi \tag{2.4}$$

which can be rearranged to

$$\Rightarrow \mathrm{d}A = \frac{r^2}{\cos\alpha} \quad \mathrm{d}\Omega \tag{2.5}$$

Thus, the solid angle is given by

$$\Omega = \int_A \frac{\mathrm{d}A \cdot \cos\alpha}{r^2} \tag{2.6}$$

The unit of the solid angle is a steradian (sr). The solid angle of an entire sphere is calculated by integration of equation (2.3) over the zenith (θ) and azimuth (ϕ) angles, $0 \leq \theta \leq \pi(180°)$ and $0 \leq \phi \leq 2\pi(360°)$, 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 2.2.

Putting all this together, the radiative transfer equation is

$$\cos\theta \frac{\mathrm{d}L}{\mathrm{d}z} = -(a+b) \cdot L + L^E + L^I + L^S \tag{2.7}$$

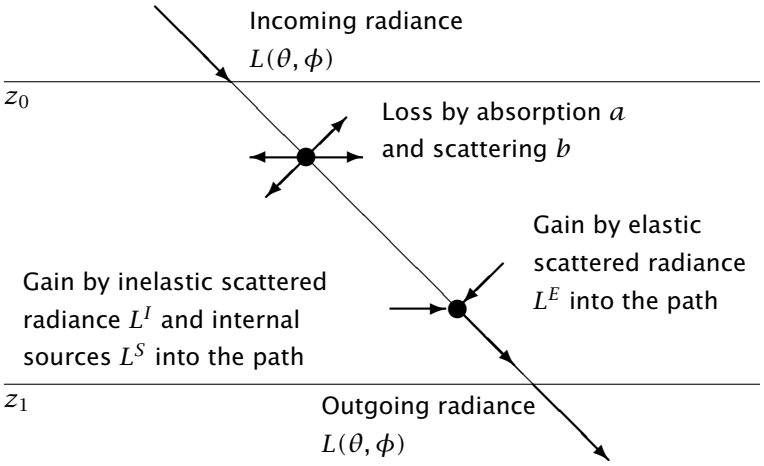


Figure 2.2: Path of the radiance and influences of absorbing and scattering particles in a thin homogeneous horizontal layer of air or water. The layer is separated from other layers of different characteristics by boundary lines at height z_0 and z_1.

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 numerical models or to make approximations and find an analytical parameterisation. 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 (Prahl et al. 1989), (Wang et al. 1995)[3], or (Mobley 1994).

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 2.7 can be integrated easily and yields

$$L(z_1) = L(z_0) \cdot \mathrm{e}^{-\frac{a \cdot (z_1 - z_0)}{\cos\theta}} \tag{2.8}$$

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.

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

Table 2.2: 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

Different physical quantities are used to describe the “amount of radiation” and their definitions and abbreviations are listed in Table 2.2. Taking into account Equation 2.6 and assuming a homogenous flux, the important correlation between irradiance E and intensity I is

$$E = \frac{I \cdot \cos\alpha}{r^2} \tag{2.9}$$

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 the figure below 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 (Schwiegerling 2004). 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 2.2, 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.

Table 2.3: 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

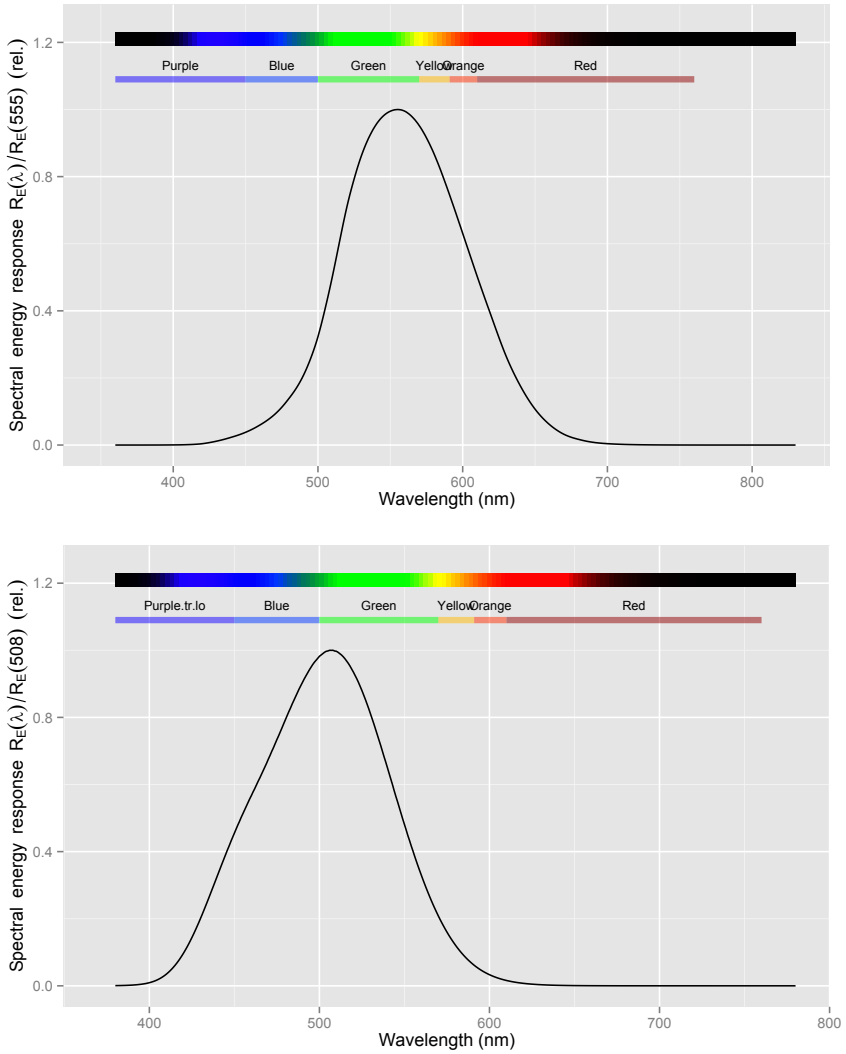


Figure 2.3: Relative spectral intensity of human colour sensation during day (solid line) and night (dashed line), $V(\lambda)$ and $V'(\lambda)$ respectively.

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 2.2, the equivalent photon related quantities are listed in the table below and have the subscript p.

Table 2.4: 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

These quantities can be also used based on a 'chemical' amount of moles by dividing the quantities by Avogadro's number $N_A = 6.022 \times 10^{23}\ \mathrm{mol}^{-1}$. 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 defined in equation 2.1. This yields for example

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

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 $4.6\ \mu\mathrm{mol\,m^{-2}\,s^{-1}}$. 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 **??**.

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

Table 2.5: Conversion factors of photon and energy quantities at different wavelengths.

	$\mathrm{W\,m^{-2}}$ to $\mu\mathrm{mol\,m^{-2}\,s^{-1}}$	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

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.

$$E_0(\lambda) = \int_\Omega L(\lambda, \Omega)\mathrm{d}\Omega \tag{2.10}$$

$$E(\lambda) = \int_\Omega L(\lambda, \Omega)|\cos\alpha|\mathrm{d}\Omega \tag{2.11}$$

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 **??**.

2.3 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 2.4 for a diagram. In contrast to Figure 2.1 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 2.4 the observer is situated at the origin.

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):

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

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'),

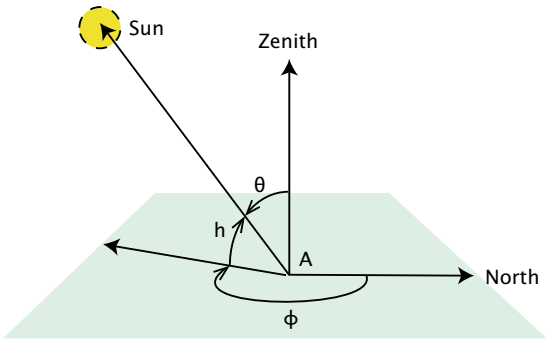


Figure 2.4: Position of the sun in the sky and the different angles used for its description by an observer located at point A. The azimuth angle is ϕ, the elevation angle is h and the zenith angle is θ. These angles are measured on two perpendicular planes, one horizontal and one vertical.

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):

$$L_s(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{e^{(hc/k_B T\lambda)} - 1} \tag{2.12}$$

with Boltzmann's constant $k_B = 1.381 \times 10^{-23}$ 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

$$\lambda_{max} \cdot T = 2.898 \times 10^6 \,\text{nm K} \tag{2.13}$$

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 $E_s(\lambda)$ can be estimated assuming a homogeneous flux and using the correlation of intensity I and radiance L from their definitions in table 2.2. The intensity of the sun $I_s(\lambda)$ is given by the radiance $L_s(\lambda)$ 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 (2.9). Thus, the extraterrestrial solar irradiance is

$$E_s(\lambda) = L_s(\lambda) \cdot \frac{\pi r_s^2}{r_0^2} \tag{2.14}$$

Remembering the solid angle of equation (2.6), 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 2.5 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.

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

Integrated over all wavelengths, E_s is about 1361 to 1362 $\mathrm{W\,m^{-2}}$ at top of the atmosphere (Kopp and Lean 2011). This value is called the 'solar constant'. In former times, depending on different measurements, E_s varies by a few percent (Iqbal 1983). 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 (Mobley 1994). 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 (Fröhlich and Lean 2004). 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

$$L = \frac{\sigma}{\pi} \cdot T^4 \tag{2.15}$$

with the Stefan-Boltzmann constant $\sigma = 5.6705 \times 10^{-8}$ W m^{-2} K^{-4}. With $T = 5800$ K equation 2.15 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 2.6 and 2.9).

Figure 2.5: Extraterrestrial solar spectrum after (Wehrli 1985) (green line) and spectrum of a black body at 5800 K (red line), calculated using Planck's law (equation 16.1) and converted to extraterrestrial spectral irradiance with equation 2.14.

The total solar irradiance covers a wide range of wavelengths. Using some of the 'colours' introduced in table 2.1, table 2.6 lists the irradiance and fraction of E_s of different wavelength intervals.

Table 2.6: Distribution of the extraterrestrial solar irradiance E_s constant in different wavelength intervals calculated using the data of (Wehrli 1985) shown in Figure 2.5.

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, 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

Figure 2.6: Sky photos in different portions of the light spectrum. They show that in the UV-A band the diffuse component is proportionally larger than it is at longer wavelengths. This can be seen as reduced contrast. Photographs taken by L. Ylianttila at the fortress of Suomenlinna (`http://www.suomenlinna.fi/en`), Helsinki, Finland.

Figure 2.7: 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 2.8: 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 (Kotilainen et al. 2011) for details about the simulations.

München (11.60° E, 48.22° N, 490 m above sea level) on two sunny days (17^{th} April 1996, sun zenith angle of 38° and 27^{th} 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 has two components, and . 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 2.6 and 2.7).

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 2.8 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 2.9) or use a logarithmic scale (Figure 2.10), 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.

Figure 2.9: The effect of ozone depletion on the UV spectrum of global (direct plus diffuse) solar radiation at noon. See fig. 2.8 for details.

Figure 2.10: 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. 2.8 for details.

Figure 2.11: UV-B and PAR. Left: Diffuse radiation as percentage of total (direct + diffuse) radiation in the UV-B (solid line) and PAR (dashed line) wavebands for open areas in a humid temperate climate under a clear sky. In cloudy conditions the percentage of diffuse radiation increases. Day of year not specified. Redrawn from (Flint and Caldwell 1998). Right: Seasonal variation in modelled, clear sky, solar-noon, UV-B (solid line) and PAR (dashed line) irradiance above the canopy for Maryland, USA. Irradiance expressed relative to annual maximum of each waveband. Adapted from (Brown et al. 1994).

Seasonal variation in UV-B irradiance has a larger relative amplitude than variation in PAR (Figure 2.11). This causes a seasonal variation in the UV-B: PAR ratio (Figure 2.12). In addition to the regular seasonal variation, there is random variation as a result of changes in clouds (Figure 2.12). 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 2.13) 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 (Flenley 1992).

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 (see Graedel and Crutzen 1993). 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 (Manney et al. 2011) 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

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

Figure 2.12: Seasonal variation in UV-B radiation at Erlangen, Germany (54° 10' N, 07° 51' E, 280 m asl). (Top) UV-B:PAR energy ratio, calculated from daily exposures, and (bottom) UV-B daily exposure, measured with ELDONET instruments (see Figure 2 in Häder et al. 2007, for details).

Figure 2.13: Latitudinal variation in UV-B radiation in the Northern hemisphere. UV-B annual exposure, measured with ELDONET instruments (see Häder et al. 2007, for details).

long half life in the 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 (Hegglin and Shepherd 2009). In addition, increased cloudiness and pollution, could lead to decreased UV and PAR, sometimes called 'global dimming' (e.g. Stanhill and Cohen 2001). It should be noted that, through reflection, broken clouds can locally increase UV irradiance to values above those under clear-sky conditions (S. B. Díaz et al. 1996; Frederick et al. 1993).

2.4 Radiation within 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 (Monsi and Saeki 1953), reviewed by (Hirose 2005). Beer's law (Equation 2.8) 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).

$$I_z = I_0 \cdot \mathrm{e}^{-K L_z} \tag{2.16}$$

Equation 2.16 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 2.11). In sunlit patches in forest gaps the diffuse radiation percentage is lower

than in open areas, because 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 (see Brown et al. 1994). In contrast, (Deckmyn et al. 2001) observed a decrease in UV:PAR ratio in white clover canopies with planophyle leaves. (Allen et al. 1975) modelled the UV-B penetration in plant canopies, under normal and depleted ozone conditions. (Parisi and Wong 1996) 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 (Grant 1998, 1999a,b, 2004).

Detailed accounts of different models describing the interaction of radiation and plant canopies, taking into account the properties of foliage, are given by (Campbell and Norman 1998) and (Monteith and Unsworth 2008).

CHAPTER 3

Photochemistry

Abstract

In this chapter we explain how to .

3.1 Task:

CHAPTER 4

Software

Abstract

In this chapter we describe the software we used to run the code examples and typeset this handbook, and how to install it. Which is basically the same we use for everyday data analysis and typesetting.h

4.1 Task:

4.2 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 (Aphalo, Albert, Björn, Ylianttila et al. 2012).

Combining R with Markdown (Rmarkdown: Rmd files) or LaTeX (Rnw fiels) 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.

4.3 The different pieces

4.3.1 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 "add-ons" 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 by using them as building blocks in our packages, and for the production of the examples. The most notable ones are: `data.table`, `lubridate`, and `ggplot2`. Packages `devtools` and `testthat` significantly easied the task of package development and coding.

If you are not familiar with R, please, go through the separately available Supplements **??**, **??**, **??**, and **??**, and/or learn from some of the books listed in Appendix **??**, before delving into our 'Cook Book'.

4.3.2 RStudio

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.

4.3.3 Version control: Git and Subversion

Version 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.

4.3.4 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.

4.3.5 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 forats, and is the most popular TeX engine in China and other Asian countries.

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

4.3.6 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 different output formats in addition to PDF.

CHAPTER 5

Photobiology R packages

Abstract

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

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 user interface

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 all observations are referenced to a wavelength value, there are different types spectral objects, e.g. for light sources and responses to light. Waveband objects include much

Figure 5.1: The elements of 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.

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.

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

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

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.

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

Is all what is needed to obtain the CIE98-weigthed 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 automatically 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

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

	Package	Type	Contents
•	photobiologyAll	dummy	loads other packages of the suite
•	photobiology	funs + classes	basic functions, class definitions, class methods and example data
•	photobiologyInOut	functions	data import/export functions
•	photobiologyWavebands	definitions	quantification of radiation
•	photobiologygg	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	functions	Ocean Optics spectrometers
•	MayaCalc	functions	UV and VIS irradiance data processing for Maya2000 Pro
•	rTUV	funs + data	TUV model interface

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 irradi-

ance `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 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

I have created a repository for the packages. This repository follows the CRAN folder structure, so package installation can be done using normal R commands. This means that dependencies are installed automatically and that automatic updates are possible. The build most suitable for the current system and R version is also picked automatically if available. It is normally recommended that you do installs and updates on a clean R session (just after starting R or RStudio). For easy installation and updates of packages, the 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"))
```

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:

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

```
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 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", "photobiologygg"))
```

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 II

Cookbook of calculations

CHAPTER 6

Storing data

Abstract

In this chapter we describe the objects used to store data and functions and operators for basic operations. We also give some examples of operating on these objects and their components using normal R functions and operators.

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(photobiologyFilters)
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.

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

Name	Variables	Attributes
generic_spct	w.length	
cps_spct	w.length, cps	
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	

6.3 Spectra

6.3.1 How are spectra stored?

For spectra the classes are a specialization of `data.table` which are in turn a specialization of `data.frame`. This means that they are *mostly* compatible with functions that operate on these classes.

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.

Except for *special* cases each spectral object holds only spectral data from a single measurement. When spectral data from more than one measurement is contained in a single object, the data for the different measurements are stored *melted*, in 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. The name used for variables containing spectral data for a given quantity have mandatory names, and are always stored using the same units. Spectral objects also carry additional information in attributes, such a text comment, sorting key, time unit used for expression, and additional attributes indicating properties such as whether reflectance is **specular** or **total**. 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 restriction 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.

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	
cps	$n\,\mathrm{s}^{-1}$	
s.e.irrad	$\mathrm{W\,m^{-2}\,nm^{-1}}$	time.unit = "second"
s.e.irrad	$\mathrm{J\,m^{-2}\,d^{-1}\,nm^{-1}}$	time.unit = "day"
s.e.irrad	varies	time.unit = *duration*
s.q.irrad	$\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$	time.unit = "second"
s.q.irrad	$\mathrm{mol\,m^{-2}\,d^{-1}\,nm^{-1}}$	time.unit = "day"
s.q.irrad	$\mathrm{mol\,m^{-2}\,nm^{-1}}$	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	$x\,\mathrm{J^{-1}\,s^{-1}\,nm^{-1}}$	time.unit = "second"
s.e.response	$x\,\mathrm{J^{-1}\,d^{-1}\,nm^{-1}}$	time.unit = "day"
s.e.response	$x\,\mathrm{J^{-1}\,nm^{-1}}$	time.unit = "exposure"
s.e.response	varies	time.unit = *duration*
s.q.response	$x\,\mathrm{mol^{-1}\,s^{-1}\,nm^{-1}}$	time.unit = "second"
s.q.response	$x\,\mathrm{mol^{-1}\,d^{-1}\,nm^{-1}}$	time.unit = "day"
s.q.response	$x\,\mathrm{mol^{-1}\,nm^{-1}}$	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	$n\,\mathrm{s}^{-1}$	

6.3.2 Spectral data assumptions

The packages' code assumes that wavelengths are always expressed in nanometres (1 nm = $1 \cdot 10^{-9}$ m). If the data to be analysed uses different units for wavelengths, e.g. Ångstrom (1 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 connversion 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 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)

##       w.length s.e.irrad
##    1:      300         1
##    2:      301         1
##   ---
## 200:      499         1
## 201:      500         1
```

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)

##      w.length s.q.irrad
##   1:      300         1
##   2:      301         1
##  ---
## 200:      499         1
## 201:      500         1
```

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")

##      w.length s.q.irrad
##   1:      300         1
##   2:      301         1
##  ---
## 200:      499         1
## 201:      500         1
```

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 irradiances 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 can create a new object of class `source_spct` by making a copy of a data frame or a data table and converting it into a source spectrum:

```
my.df <- data.frame(w.length = 300:500, s.e.irrad = 1)
my.spct <- as.source_spct(my.df)
```

In this case `sun.data` remains independent, and whatever change we make to my.spct does not affect `sun.data`:

```
my.spct <- my.spct * 2
my.spct

##       w.length s.e.irrad
##    1:      300         2
##    2:      301         2
##   ---
## 200:      499         2
## 201:      500         2

head(my.df)

##   w.length s.e.irrad
## 1      300         1
## 2      301         1
## 3      302         1
## 4      303         1
## 5      304         1
## 6      305         1
```

These functions, in the same way as constructors, accept attributes as arguments.

Using a technical term, we have used a copy constructor, which is the normal behaviour in R.

6.3.5 Task: Convert a data frame into a spectral object

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

or data table, *in situ* or by reference, into a `source_spct` object. These `set` functions 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.

```
my.ref.spct <- setSourceSpct(my.df)
is.source_spct(my.df)

## [1] TRUE
```

If we combine the above code with an assignment, we end up having two names for the *same* object, which has been converted to a `source_spct` object. (At the moment we get a copy!)

```
my.ref.spct <- my.ref.spct * 2
my.ref.spct

##      w.length s.e.irrad
##   1:      300         2
##   2:      301         2
##  ---
## 200:      499         2
## 201:      500         2

my.df

##      w.length s.e.irrad
##   1:      300         1
##   2:      301         1
##  ---
## 200:      499         1
## 201:      500         1
```

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

```
setSourceSpct(my.df)
```

These functions, in the same way as constructors, accept attributes as arguments.

Using a technical term, we have converted an object by *reference*, which is *not* the normal behaviour in R.[1]

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

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

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_spct(sun.spct, range = UV())

## Warning in trim_spct(sun.spct, range = UV()): Not trimming
short end as low.limit is outside spectral data range.

##       w.length    s.e.irrad    s.q.irrad
##    1:      293 2.609665e-06 6.391730e-12
##    2:      294 6.142401e-06 1.509564e-11
##   ---
## 107:      399 5.861190e-01 1.954901e-06
## 108:      400 6.081049e-01 2.033314e-06

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

##       w.length s.e.irrad s.q.irrad
##    1:      100         0         0
##    2:      101         0         0
##   ---
## 701:      799         0         0
## 702:      800         0         0

trim_spct(sun.spct, low.limit = 400)

##       w.length s.e.irrad    s.q.irrad
##    1:      400 0.6081049 2.033314e-06
##    2:      401 0.6261742 2.098967e-06
##   ---
## 400:      799 0.4185850 2.795738e-06
## 401:      800 0.4069055 2.721132e-06

trim_spct(sun.spct, low.limit = 250, fill = 0.0)

##       w.length s.e.irrad    s.q.irrad
##    1:      250 0.0000000 0.000000e+00
##    2:      251 0.0000000 0.000000e+00
##   ---
## 550:      799 0.4185850 2.795738e-06
## 551:      800 0.4069055 2.721132e-06

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

##       w.length   s.e.irrad    s.q.irrad
##    1:      300 0.001264554 3.171207e-09
##    2:      301 0.002623718 6.601607e-09
##   ---
## 300:      599 0.624741526 3.128191e-06
## 301:      600 0.637276746 3.196284e-06
```

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_spct(sun.spct, range=c(300, 1000))

## Warning in trim_spct(sun.spct, range = c(300, 1000)): Not
trimming long end as high.limit is outside spectral data range.

##      w.length   s.e.irrad    s.q.irrad
##   1:      300 0.001264554 3.171207e-09
##   2:      301 0.002623718 6.601607e-09
##  ---
## 500:      799 0.418584959 2.795738e-06
## 501:      800 0.406905530 2.721132e-06

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

##      w.length s.e.irrad s.q.irrad
##   1:      293        NA        NA
##   2:      294        NA        NA
##  ---
## 708:      999        NA        NA
## 709:     1000        NA        NA

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

##      w.length s.e.irrad s.q.irrad
##   1:      293         0         0
##   2:      294         0         0
##  ---
## 708:      999         0         0
## 709:     1000         0         0
```

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 NAs unless a different argument is provided for parameter `fill`:

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

##      w.length   s.e.irrad    s.q.irrad
##   1:    290.0          NA           NA
##   2:    290.1          NA           NA
```

```
##  ---
## 100:    299.9 0.001216553 3.050176e-09
## 101:    300.0 0.001264554 3.171207e-09

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

##      w.length   s.e.irrad    s.q.irrad
##   1:    290.0 0.000000000 0.000000e+00
##   2:    290.1 0.000000000 0.000000e+00
##  ---
## 100:    299.9 0.001216553 3.050176e-09
## 101:    300.0 0.001264554 3.171207e-09
```

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

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

##      w.length   Tfr
##   1:    290.0 0.004
##   2:    290.1 0.004
##  ---
## 100:    299.9 0.003
## 101:    300.0 0.003
```

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, and its reimplementation from package `data.table`, and function `rbindlist` also defined in package `data.table` 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 <- copy(sun.spct)
```

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

```
##       w.length    s.e.irrad    s.q.irrad
##    1:      293 2.609665e-06 6.391730e-12
##    2:      293 2.609665e-06 6.391730e-12
##   ---
## 1015:      800 4.069055e-01 2.721132e-06
## 1016:      800 4.069055e-01 2.721132e-06
```

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)

##       w.length    s.e.irrad spct.idx    s.q.irrad
##    1:      293 2.609665e-06        A 6.391730e-12
##    2:      294 6.142401e-06        A 1.509564e-11
##   ---
## 1015:      799 4.185850e-01        B 2.795738e-06
## 1016:      800 4.069055e-01        B 2.721132e-06
```

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)

##       w.length    s.e.irrad spct.idx    s.q.irrad
##    1:      293 2.609665e-06      sun 6.391730e-12
##    2:      294 6.142401e-06      sun 1.509564e-11
##   ---
## 1015:      799 4.185850e-01    shade 2.795738e-06
## 1016:      800 4.069055e-01    shade 2.721132e-06
```

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")

##       w.length    s.e.irrad    ID    s.q.irrad
##    1:      293 2.609665e-06   sun 6.391730e-12
##    2:      294 6.142401e-06   sun 1.509564e-11
##   ---
## 1015:      799 4.185850e-01 shade 2.795738e-06
## 1016:      800 4.069055e-01 shade 2.721132e-06
```

6.4 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.

6.5 Wavebands

6.5.1 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.

6.5.2 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) 293
## 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].

[2] It is preferable that `wb.name` complies with the requirements for R object names and file

```
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 85, 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")

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

See chapter 11 on page 105, in particular sections **??**, **??**, and **??** for further examples, and a more in-depth discussion of the creation and use of *weighted* `waveband` objects.

6.5.3 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

names, while labels have fewer restrictions as they are meant to be used only for output text labels.

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_waveband(UV(), range = UVB())

## [[1]]
## UV.ISO.tr.lo.hi
## low (nm) 280
## high (nm) 315
## weighted none

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

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

trim_waveband(VIS_bands(), low.limit = 400, trim = TRUE)

## [[1]]
## Purple.ISO.tr.lo
## low (nm) 400
## 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_waveband(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:photobiologyFilters))
try(detach(package:photobiology))
```

CHAPTER 7

Math operators and functions

Abstract

In this chapter we describe math functions and operators for spectra and wavebands. Many of these are specializations of the generic operators and functions existing in R.

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.

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

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

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.new.spct

##      w.length    s.e.irrad
##   1:      293 7.828995e-09
##   2:      294 1.842720e-08
##  ---
## 507:      799 3.809123e-01
## 508:      800 3.706909e-01
```

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

##      w.length    s.e.irrad
##   1:      293 1.304833e-06
##   2:      294 3.071200e-06
##  ---
## 507:      799 2.092925e-01
## 508:      800 2.034528e-01

2 * sun.spct

##      w.length    s.e.irrad
##   1:      293 5.219330e-06
##   2:      294 1.228480e-05
##  ---
## 507:      799 8.371699e-01
## 508:      800 8.138111e-01

sun.spct * 2

##      w.length    s.e.irrad
##   1:      293 5.219330e-06
##   2:      294 1.228480e-05
##  ---
## 507:      799 8.371699e-01
## 508:      800 8.138111e-01
```

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)

##      w.length  s.e.irrad
##   1:      293 -5.5834152
##   2:      294 -5.2116619
##  ---
## 507:      799 -0.3782164
## 508:      800 -0.3905064
```

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.

```
filtered_sun.spct <- sun.spct * gg400.spct
filtered_sun.spct

##      w.length    s.e.irrad
##   1:      293 2.609665e-11
##   2:      294 6.142401e-11
##  ---
## 507:      799 4.060274e-01
## 508:      800 3.946984e-01
```

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

```
filtered_uncoated_sun.spct <- sun.spct * gg400.spct * (100 - 9) / 100
filtered_uncoated_sun.spct

##      w.length    s.e.irrad
##   1:      293 2.374795e-11
##   2:      294 5.589585e-11
##  ---
## 507:      799 3.694849e-01
## 508:      800 3.591755e-01
```

Calculations related to filters will be explained in detail in chapter **??**. 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

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06

sun.spct * 2

##      w.length    s.e.irrad
##   1:      293 5.219330e-06
##   2:      294 1.228480e-05
##  ---
## 507:      799 8.371699e-01
## 508:      800 8.138111e-01
```

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)
```

As spectral objects are derived from `data.table`, it is also possible to use data table syntax, returning a vector:

```
# not run
sun.spct[ , s.e.irrad^2 / w.length]
```

or, adding the result to the spectral object—in this case we need to first copy `sun.spct`, because it is protected because it is part of a package:

```
# run
my_sun.spct <- copy(sun.spct)
my_sun.spct[ , result := s.e.irrad^2 / w.length]

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06
##             result
##   1: 2.324352e-14
##   2: 1.283302e-13
##  ---
## 507: 2.192908e-04
## 508: 2.069651e-04

my_sun.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
```

```
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06
##            result
##   1: 2.324352e-14
##   2: 1.283302e-13
##  ---
## 507: 2.192908e-04
## 508: 2.069651e-04
```

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 vectorized, 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, there is no internal check that the wavelength values agree at each element. So, although such code may execute faster, it is not recommended in normal use.

Operations using built-in R operators cannot be used if the wavelengths in two spectral data sets are not matched. In this situation functions and operators defined in package `photobiology` come to the rescue by transparently making the two operand spectra compatible by interpolation. The result they return includes all the individual wavelength values (the set union of the wavelengths from the two spectra in the region where they overlap). The functions are `sum_spectra`, `subt_spectra`, `prod_spectra`, `div_spectra`, and `oper_spectra`. Here is a very simple hypothetical example:

```
# not run
out1.dt <- sum_spectra(spc1$w.length, spc2$w.length,
                       spc1$s.e.irrad, spc2$s.e.irrad)
```

However, we can achieve the same result, with simpler syntax, using spectral objects and the corresponding operators. The actual computations are done in both cases by the same code, but the example below adds some "syntactic sugar" to make the script code more readable.

```
out2.spct <- sun.spct + sun.spct
out2.spct

##      w.length    s.e.irrad
##   1:      293 5.219330e-06
##   2:      294 1.228480e-05
##  ---
## 507:      799 8.371699e-01
## 508:      800 8.138111e-01
```

```
out3.spct <- e2q(sun.spct + sun.spct)
out3.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 5.219330e-06 1.278346e-11
```

```
##   2:       294 1.228480e-05 3.019128e-11
##  ---
## 507:       799 8.371699e-01 5.591475e-06
## 508:       800 8.138111e-01 5.442264e-06
```

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. `out1.data` is a `data.table` while `out2.data` and `out3.data` are `source_spct`. The class of the returned spectrum depends on the classes of the operands.

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:

[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.

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

## [1] 919.5147
```

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

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

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

##  [1] 2.609665e-06 6.142401e-06 2.176175e-05
##  [4] 6.780119e-05 1.533491e-04 3.669677e-04
##  [7] 7.845430e-04 1.264554e-03 2.623718e-03
## [10] 3.922583e-03

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

##  [1] 6.391730e-12 1.509564e-11 5.366385e-11
##  [4] 1.677626e-10 3.807181e-10 9.141345e-10
##  [7] 1.960893e-09 3.171207e-09 6.601607e-09
## [10] 9.902505e-09
```

`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.

```
sun.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06

my_sun.spct <- copy(sun.spct)
e2q(my_sun.spct)

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06
```

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

```
sun.spct
```

```
##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06

my_sun.spct <- copy(sun.spct)
e2q(my_sun.spct, "replace")

##      w.length    s.q.irrad
##   1:      293 6.391730e-12
##   2:      294 1.509564e-11
##  ---
## 507:      799 2.795738e-06
## 508:      800 2.721132e-06

my_sun.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06
```

`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 Aphalo, Albert, Björn, Ylianttila et al. 2012 it is written: "Example 1: red light at 600 nm has about 200 $\mathrm{kJ\,mol^{-1}}$, therefore, 1 µmol photons has 0.2 J. Example 2: UV-B radiation at 300 nm has about 400 $\mathrm{kJ\,mol^{-1}}$, 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 $\mathrm{J\,mol^{-1}}$ we multiply the result by 10^{-3} to obtain $\mathrm{kJ\,mol^{-1}}$:

```
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.

```
sun.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06

my_sun.spct <- copy(sun.spct)
q2e(my_sun.spct, "replace")

##      w.length    s.e.irrad
##   1:      293 2.609665e-06
##   2:      294 6.142401e-06
##  ---
## 507:      799 4.185850e-01
## 508:      800 4.069055e-01
```

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.

```
q2e(my_sun.spct, byref=TRUE)

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06

my_sun.spct

##      w.length    s.e.irrad    s.q.irrad
##   1:      293 2.609665e-06 6.391730e-12
##   2:      294 6.142401e-06 1.509564e-11
##  ---
## 507:      799 4.185850e-01 2.795738e-06
## 508:      800 4.069055e-01 2.721132e-06
```

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 `data.table`		
datatable.print.nrows	$n = 100$	nrow(*spct*) $> n$ short" printing
datatable.print.topn	$n = 5$	nrows to print at top and bottom
datatable.verbose	FALSE	give verbose output or not
R4photobioloy suite		
photobiology.radiation.unit	`"energy"`	output ($\mathrm{W\,m^{-2}\,nm^{-1}}$)
	`"photon"`	output ($\mathrm{mol\,m^{-2}\,s^{-1}\,nm^{-1}}$)
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

`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 `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()

##     w.length    s.q.irrad
```

```
##  1:  293.000 6.391730e-12
##  2:  294.000 1.509564e-11
## ---
## 22:  314.000 2.766867e-07
## 23:  314.999 2.969737e-07

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

##     w.length    s.e.irrad
##  1:  293.000 2.609665e-06
##  2:  294.000 6.142401e-06
## ---
## 22:  314.000 1.054126e-01
## 23:  314.999 1.127828e-01
```

For filters, an option controls whether transmittance, the default, or absorbance is use in the operations, and returned.

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

##      w.length          A
##   1:      190 3.91721463
##   2:      191 4.00000000
##  ---
## 610:      799 0.08191722
## 611:      800 0.08096325

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

##      w.length      Tfr
##   1:      190 0.000121
##   2:      191 0.000100
##  ---
## 610:      799 0.828100
## 611:      800 0.829921
```

Either option can be unset, by means of the NULL value.

```
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 for performance vs. precision of calculations and can be useful especially when processing huge numbers of spectra. Some options defined in base R and package `data.table` affect printing of output.

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 6.5.3.

```
is_effective(UVA())

## [1] FALSE

sun.spct * UVA()

##     w.length s.e.irrad
##  1:  315.000 0.1127901
##  2:  316.000 0.1020587
## ---
## 85:  399.000 0.5861190
## 86:  399.999 0.6080829
```

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()

##      w.length    s.e.irrad
##   1:  293.000 2.609665e-06
##   2:  294.000 6.142401e-06
##  ---
## 107:  399.000 7.378801e-05
## 108:  399.999 7.395674e-05
```

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

CHAPTER 8

Spectra: simple summaries and features

Abstract

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

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(photobiologygg)
library(photobiologyLamps)
library(photobiologyFilters)
library(photobiologyReflectors)
```

8.2 Task: Printing spectra

Spectral objects are printed with the `print` method for `data.frame` objects, consequently, it is possible to use options from package `data.frame` to control printing. The first option set below, `datatable.print.nrows`, determines the number of rows above which only 'head' and 'tail' rows are printed. The second option, `datatable.print.topn`, determines how many rows are printed when not all rows are printed.

```
options(datatable.print.nrows = 10)
options(datatable.print.topn = 2)
```

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)

## wavelength ranges from 293 to 800 nm
## largest wavelength step size is 1 nm
## spectral irradiance ranges from 2.61e-06 to 0.8205 W m-2 nm-1
## energy irradiance is 269.1 W m-2
## spectral photon irradiance ranges from 6.392e-06 to 3.375 umol s-1 m-2 nm-1
## photon irradiance is 1255 umol s-1 m-2
```

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
## 5.308183e-01 2.476007e-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] 293 800

midpoint(sun.spct)

## [1] 546.5

max(sun.spct)

## [1] 800

min(sun.spct)

## [1] 293
```

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

```
spread(sun.spct)

## [1] 507

stepsize(sun.spct)

## [1] 1 1
```

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" "data.table"
## [4] "data.frame"

class(polyester.new.spct)
```

```
## [1] "filter_spct"  "generic_spct" "data.table"
## [4] "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.new.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.new.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.new.spct)

## [1] FALSE
```

```
is.filter_spct(sun.spct)

## [1] FALSE

is.filter_spct(polyester.new.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)

## Warning in setTimeUnit(new.spct, time.unit.spct):
Overrriding existing 'time.unit' 'second' with 'unknown' may
invalidate data!

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.new.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)

##    w.length    s.e.irrad    s.q.irrad
## 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
## 6:      298 3.669677e-04 9.141345e-10

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

##    w.length    s.q.irrad
## 1:      293 6.391730e-12
## 2:      294 1.509564e-11
## 3:      295 5.366385e-11
## 4:      296 1.677626e-10
## 5:      297 3.807181e-10
## 6:      298 9.141345e-10

is_energy_based(my.spct)

## [1] FALSE

is_photon_based(my.spct)

## [1] TRUE
```

We now consider `filter_spct` objects.

```
is_transmittance_based(polyester.new.spct)

## [1] TRUE

is_absorbance_based(polyester.new.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
```

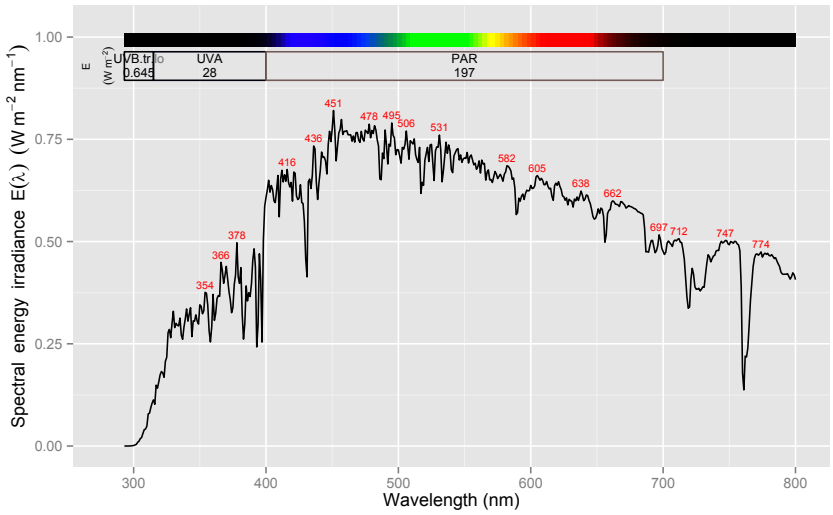
`source_spct` objects can be queried to learn if they are the result of a calculation involving a weighting function.

```
is_effective(sun.spct)

## [1] FALSE
```

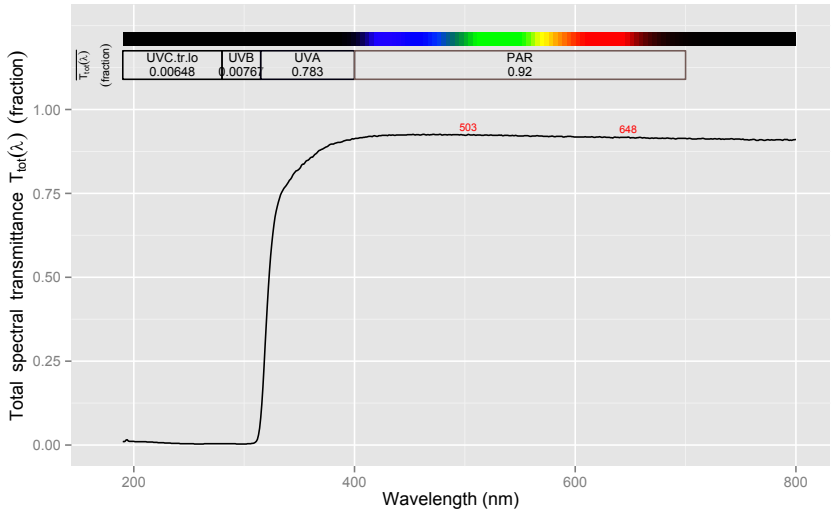
8.11 Task: Plotting a spectrum

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.new.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.

```
names(sun.spct)

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

comment(sun.spct)

## NULL
```

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)

##     w.length s.e.irrad
##  1:      313   0.29181
##  2:      365   0.06587
## ---
## 29:      691   0.00191
## 30:      730   0.00153

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

```
##     w.length    s.q.irrad
##  1:      313 7.635026e-07
##  2:      365 2.009771e-07
## ---
## 30:      691 1.103259e-08
## 31:      730 9.336418e-09

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

## span increased to next odd value:  51
##     w.length s.e.irrad
##  1:      313   0.29181
##  2:      365   0.06587
##  3:      404   0.15675
##  4:      435   0.38773
##  5:      492   0.00154
##  6:      545   0.16449
##  7:      578   0.03238
##  8:      612   0.00131
##  9:      691   0.00191
## 10:      730   0.00153
```

```
valleys(kg5.spct)

##    w.length     Tfr
## 1:      530 0.87000
## 2:     3000 0.00018

peaks(kg5.spct, filter.qty = "absorbance")

##    w.length          A
## 1:      530 0.06048075
## 2:     3000 3.74472749
```

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] 23 25 29 35 38 40
```

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 chracter 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
```

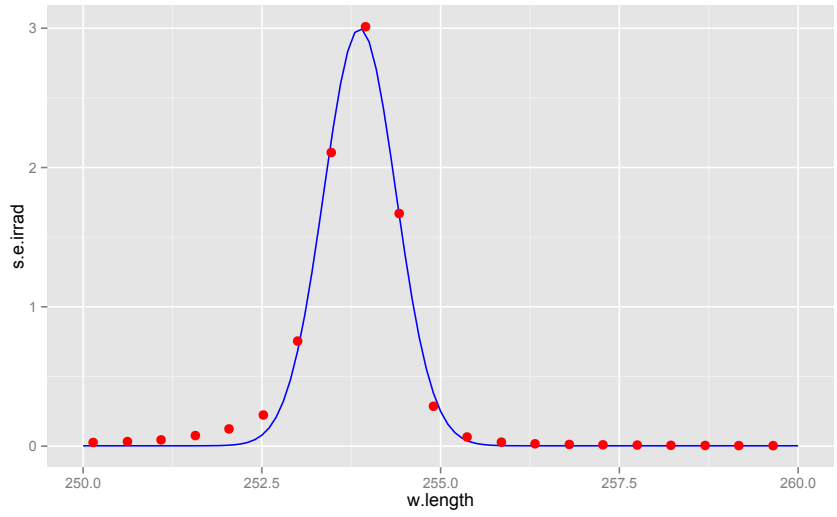
```
peaks[1, 1]

## [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:photobiologygg))
try(detach(package:photobiology))
```

CHAPTER 9

Wavebands: simple summaries and features

Abstract

In this chapter we explain how to obtain different summaries and query features from wavebands.

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(photobiologygg)
```

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] 379.9999 380.0000 759.9999 760.0000
##
## $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: 0x0000000017fecd58>
## <environment: namespace:photobiologyWavebands>
```

```
##
## $SWF.q.fun
## function (w.length)
## {
##     SWF.e.fun(w.length) * SWF.norm/w.length
## }
## <bytecode: 0x0000000017ce75b0>
## <environment: 0x00000000176129e0>
##
## $SWF.norm
## [1] 298
##
## $norm
## [1] 298
##
## $hinges
## [1] 249.999 250.000 298.000 328.000 400.000
## [6] 400.001
##
## $name
## [1] "CIE98.298"
##
## $label
## [1] "CIE98"
```

9.3 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.

```
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 *effecctive 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.

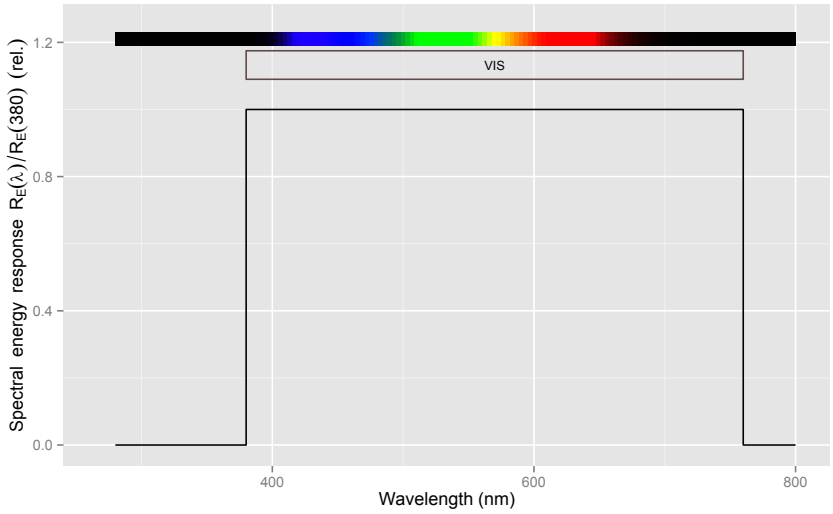
```
names(vis.wb)

##  [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"
```

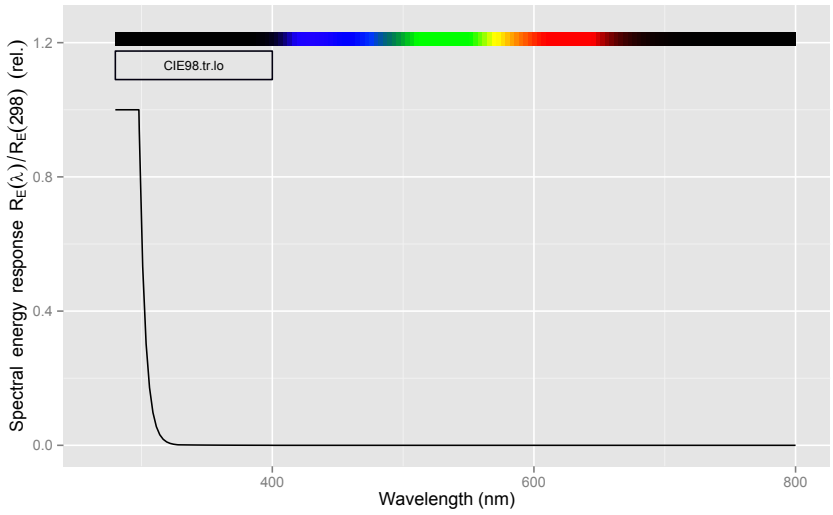
9.7 Task: Plotting a waveband

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

CHAPTER 10

Unweighted irradiance

Abstract

In this chapter we explain how to calculate unweighted energy and photon irradiances from spectral 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)
```

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 93 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 87

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)

## $CMF
##   Red.CMF
## "#900000"
##
## $CC
##    Red.CC
## "#FF0000"
```

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

```
UVB()

## 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
```

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

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.tr.lo
##      0.6445035
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

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

##  UVB.none.tr.lo
##        1.337169
## 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.tr.lo
##      0.4819911
## 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 `wavebands` 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) 293
## 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
##       68.48951
## 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
##   68.48951
## 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.293.462
## low (nm) 293
## high (nm) 462
## weighted none
##
## $wb2
```

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

```
## range.462.631
## low (nm) 462
## high (nm) 631
## weighted none
##
## $wb3
## range.631.800
## low (nm) 631
## 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
##
## $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
##
```

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

```
## [[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 $\lambda_1 = 400$nm and $\lambda_1 = 700$nm. In this example we will use example data for sunlight to calculate $E_{400\,\mathrm{nm}<\lambda<700\,\mathrm{nm}}$. 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
##              28.62868
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"

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

## 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.tr.lo        UVA.ISO
##      0.6445035     27.9841813
## 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
## 196.7004

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

##       PAR
## 196.7004
```

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
## 196.7004
```

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 10.1 and 7.2 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 $E_{400\,\mathrm{nm}<\lambda<700\,\mathrm{nm}}$. 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 $\mu mol\,m^{-2}\,s^{-1}$ 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
## 893.7598

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

##      PAR
## 893.7598
```

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

10.8 Task: irradiances for more than one waveband

As discussed above, it is possible to calculate simultaneously the irradiances 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
##   451.1084   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
## 451.1084

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
##   451.1084   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.tr.lo
##       1.675344
## 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
##   79.38161   49.26861   37.55208
## 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
## 79.61176 49.30478 37.57760
```

10.9 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]:

$$\zeta = \frac{Q_{655\text{nm}<\lambda<665\text{nm}}}{Q_{725\text{nm}<\lambda<735\text{nm}}} \tag{10.3}$$

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)
##                          1.266705
## 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()))
```

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

```
##  UVB.ISO.tr.lo: UV.ISO.tr.lo(q:q)
##                         0.01936927
##       UVB.ISO.tr.lo: VIS.ISO(q:q)
##                         0.00154142
## attr(,"radiation.unit")
## [1] "q:q ratio"
```

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

##    Red.ISO: VIS.ISO(q:q)  Green.ISO: VIS.ISO(q:q)
##                 0.4150476                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)
##                 0.15087805
##    Blue.ISO: VIS.ISO(q:q)
##                 0.13711570
##   Green.ISO: VIS.ISO(q:q)
##                 0.20259363
##  Yellow.ISO: VIS.ISO(q:q)
##                 0.06106050
##  Orange.ISO: VIS.ISO(q:q)
##                 0.05545497
##     Red.ISO: VIS.ISO(q:q)
##                 0.41504763
## 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] 1.275899
```

or using the predefined convenience function `R_FR_ratio`:

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

## [1] 1.275899
```

10.10 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)
##                          1.401143
## attr(,"radiation.unit")
## [1] "e:e ratio"
```

other examples in section 10.9 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] 1.411385
```

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

10.11 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:

$$\bar{q}' = \frac{Q_{\lambda_1<\lambda<\lambda_2}}{E_{\lambda_1<\lambda<\lambda_2}} \tag{10.4}$$

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)
##     3.433901e-06     3.968590e-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] 4.543762e-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] 4.543762
```

10.12 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
##       69.69042       68.48951       58.45435
## 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
##       69.69042       68.48951       58.45435
## 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
##       69.69042       68.48951       58.45435
## 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
##      0.3544164      0.3483091      0.2972745
## 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
##      0.3544164      0.3483091      0.2972745
## 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
##       69.69042       68.48951       58.45435
## 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
##       69.69042       68.48951       58.45435
## 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
##      69.63243      68.53291      58.53508
```

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
##     0.3540024     0.3484126     0.2975849
```

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
##      35.40024      34.84126      29.75849
```

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
##      35.40024      34.84126      29.75849
```

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

## range.400.500 range.500.600
##       50.3979       49.6021
```

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
##      196.7004
```

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

CHAPTER 11

Weighted and effective irradiance

Abstract

In this chapter we explain how to calculate weighted energy and photon irradiances from spectral 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)
```

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. The current package makes 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
##        0.1028376
## 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
##       0.02397115
## 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
##       0.08177754
## 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
##        0.1028376        0.1473586
## 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
##       0.02397115       0.10283765
## 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
##     2.578929e-07
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

11.8 Task: calculate daily effective energy exposure

To calculate daily exposure values, we need to apply the same code as used above, but using 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 uints 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"`).

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

CHAPTER 12

Transmission and reflection

Abstract

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

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

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 defines generic functions and specialized functions, that can be used on vectors and on `filter_spct` objects. Then 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 follows.

```
my_gg400.spct <- copy(gg400.spct)
my_gg400.spct[ , A := T2A(Tfr)]

##       w.length   Tfr A
##    1:      200 1e-05 5
##    2:      210 1e-05 5
##   ---
## 179:     5100 1e-05 5
## 180:     5150 1e-05 5

my_gg400.spct

##       w.length   Tfr A
##    1:      200 1e-05 5
##    2:      210 1e-05 5
##   ---
## 179:     5100 1e-05 5
## 180:     5150 1e-05 5
```

12.4 Task: spectral absorbance from spectral transmittance

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

```
my_gg400.spct <- copy(gg400.spct)
T2A(my_gg400.spct)

##      w.length   Tfr A
##   1:      200 1e-05 5
##   2:      210 1e-05 5
##  ---
## 179:     5100 1e-05 5
## 180:     5150 1e-05 5

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

12.5 Task: spectral transmittance from spectral absorbance

```
A2T(a.gg400.spct)

##      w.length A   Tfr
##   1:      200 5 1e-05
##   2:      210 5 1e-05
##  ---
## 179:     5100 5 1e-05
## 180:     5150 5 1e-05

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

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

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" "data.table"
## [4] "data.frame"

class(gg400.spct)

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

```
my_sun.spct <- copy(sun.spct)
my_gg400.spct <- copy(gg400.spct)
filtered_sun.spct <- sun.spct * gg400.spct
class(filtered_sun.spct)

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

head(filtered_sun.spct)

##    w.length    s.e.irrad
## 1:      293 2.609665e-11
## 2:      294 6.142401e-11
## 3:      295 2.176175e-10
## 4:      296 6.780119e-10
## 5:      297 1.533491e-09
## 6:      298 3.669677e-09
```

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

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

##  UV.ISO.tr.lo
##      86.49495
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(my_sun.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      86.49495
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(filtered_sun.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      3.651128
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"

q_irrad(sun.spct * gg400.spct, UV()) * 1e6

##  UV.ISO.tr.lo
##      3.651128
## 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
##      3.651128
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

```
q_irrad(my_sun.spct * my_gg400.spct) * 1e6

##    Total
## 1135.601
## 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.293.800
##       1135.601
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

Remember, thet 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 individaul light source. If we want then to add the effect of a filter we must multiply by the filter transmittance.

> In the current version of package `photobiology` the operator is "chosen" based on the first operand. For this reason, when including a numeric operand, it should always be the second operand of binary operators for spectra.

```
# not working
my_luminaire <-
  (0.5 * Norlux_B.spct + Norlux_R.spct) *  PLX0A000_XT.spct
my_luminaire

##       w.length s.e.irrad
##    1:   200.00         0
##    2:   200.47         0
##   ---
## 2358:   937.00         0
## 2359:   937.34         0

# works fine
my_luminaire <-
  (Norlux_B.spct * 0.5 + Norlux_R.spct) *  PLX0A000_XT.spct
my_luminaire
```

```
##       w.length s.e.irrad
##    1:   200.00         0
##    2:   200.47         0
##   ---
## 2358:   937.00         0
## 2359:   937.34         0

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))
```

CHAPTER 13

Astronomy

Abstract

In this chapter we explain how to code some astronomical computations in R.

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)

##
## Attaching package:  'lubridate'
##
## The following objects are masked from 'package:data.table':
##
##    hour, mday, month, quarter, wday, week,
##    yday, year

library(ggplot2)
library(ggmap)
```

13.2 Introduction

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 UTC"

ymd("2014-03-20")

## [1] "2014-03-20 UTC"

ymd("14-03-20")

## [1] "2014-03-20 UTC"

ymd("2014-3-20")

## [1] "2014-03-20 UTC"

ymd("2014/3/20")

## [1] "2014-03-20 UTC"

dmy("20.03.2014")

## [1] "2014-03-20 UTC"

dmy("20032014")

## [1] "2014-03-20 UTC"

mdy("03202014")

## [1] "2014-03-20 UTC"
```

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.

For astronomical calculations we also need as argument the geographical coordinates. It is, of course, possible to enter latitude and longitude values recorded with a GPS instrument or manually obtained from a map. However, when the location is searchable through Google Maps, it is also possible to obtain the coordinates by means of a query from within R using packages `RgoogleMaps`, or package `ggmap`, as done here. When inputing 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).

```
geocode("Helsinki")

##        lon      lat
## 1 24.94102 60.17332
```

```
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 vectorized for the `date` parameter.

Northern hemisphere latitudes are given as positive numbers and Southern hemisphere latitudes are given as negative numbers, in degrees, possibly with decimal fractions. The default date is `today`.

```
day_length(lat =  60, lon = 0)

## [1] 18.4765

day_length(lat = -60, lon = 0)

## [1] 5.526935
```

Longitudes can be given similarly, with East of Greenwich being negative and West of Greenwhich positive.

Function `geocode` from package `ggmap` returns suitable values in a `data.frame` based on search term(s). It uses Google to do the search, so some use restrictions apply.

```
my.city <- geocode('helsinki')
my.city

##        lon      lat
## 1 24.94102 60.17332
```

We can calculate the photoperiod for the current day as

```
day_length(lon = my.city$lon, lat = my.city$lat)

## [1] 18.53689
```

Or also give a date explicitly using functions from package `lubridate`.

```
day_length(ymd("2015-06-09", tz = "EET"),
           lon = my.city$lon, lat = my.city$lat)

## [1] 18.33841

day_length(dmy("9.6.2015", tz = "EET"),
           lon = my.city$lon, lat = my.city$lat)

## [1] 18.33841
```

The complementary function `night_length` gives

```
night_length(ymd("2015-06-09", tz = "EET"),
             lon = my.city$lon, lat = my.city$lat)

## [1] 5.661595
```

It is also possible to use a vector of dates, for example created as a sequence in the next chunk using functions from package `lubridate`.

Default time zone of `ymd` is UTC or GMT, but one should set the same time zone as will be used for further calculations.

```
dates <- seq(from = ymd("2015-01-01", tz = "EET"),
             to = ymd("2015-12-31", tz = "EET"),
             by = "7 day")
photoperiods.df <-
  data.frame(date = dates,
             photoperiod = day_length(dates,
                                      lon = my.city$lon,
                                      lat = my.city$lat))
```

The 10 lines at the top of the output are

```
head(photoperiods.df, 10)

##          date photoperiod
## 1  2015-01-01    5.630232
## 2  2015-01-08    5.930886
## 3  2015-01-15    6.347161
## 4  2015-01-22    6.849658
## 5  2015-01-29    7.412069
## 6  2015-02-05    8.013514
## 7  2015-02-12    8.638686
## 8  2015-02-19    9.277017
## 9  2015-02-26    9.921603
## 10 2015-03-05   10.568204
```

A further option described in section 13.4 allow setting the twilight angle to be used for the day length calculations.

13.4 Task: Calculating times of sunrise, solar noon and sunset

Functions `sunrise_time`, `sunset_time`, and `noon_time` have all the same parameter signature.

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"`. 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.

The default for `date` is the current day in time zone UTC.

```
sunrise_time(lat = 60)

## [1] "2015-06-18 02:46:52 UTC"
```

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] "2015-06-18 02:46:52 UTC"

sunrise_time(today(tz = "EET"), lat = 60, lon = 25, tz = "EET")

## [1] "2015-06-18 04:06:53 EEST"
```

Finally 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 = "EET"), lat = 60, lon = 25, tz = "EET",
             twilight = "civil")

## [1] "2015-06-18 02:10:18 EEST"

sunrise_time(today(tzone = "EET"), lat = 60, lon = 25, tz = "EET",
             twilight = -10)

## [1] NA

sunrise_time(today(tzone = "EET"), lat = 60, lon = 25, tz = "EET",
             twilight = +12)

## [1] "2015-06-18 06:12:04 EEST"
```

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 = dates,
             sunrise_at =
               sunrise_time(dates,
                            lon = my.city$lon, lat =  my.city$lat,
                            tz = "EET", unit.out = "hour"))
```

The 10 lines at the top of the output are

```
head(time_at_sunrise.df, 10)

##          date sunrise_at
## 1  2015-01-01   9.580854
## 2  2015-01-08   9.484315
## 3  2015-01-15   9.322946
## 4  2015-01-22   9.109335
## 5  2015-01-29   8.855265
## 6  2015-02-05   8.570562
## 7  2015-02-12   8.262970
## 8  2015-02-19   7.938459
## 9  2015-02-26   7.601642
## 10 2015-03-05   7.256146
```

Functions `day_night` from our `photobiology` package uses function `sun_angles`, which is a modified version of function `sunAngle` from package `ode`, to calculate the elevation of the sun. We first find local solar noon by finding the maximal solar elevation, and then search for sunrise in the first half of the day and for sunset in the second half, defined based on the local solar noon. Sunset and sunrise are by default based on a solar elevation angle equal to zero. The argument `twilight` can be used to set the angle according to different conventions.

In the examples we use `geocode` to get the latitude and longitude of cities. `geocode` accepts any valid Google Maps search terms, including street addresses, and postal codes within cities. `day_length` returns a numeric vector. This first example is 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.

```
geo_code_BA <- geocode("Buenos Aires")
day_night(ymd("2013-12-21"),
          lon = geo_code_BA[["lon"]],
          lat = geo_code_BA[["lat"]],
          tz = "America/Argentina/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
```

And with `unit.out` set to `"hour"`

```
day_night(ymd("2013-12-21"),
          lon = geo_code_BA[["lon"]],
          lat = geo_code_BA[["lat"]],
          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:

```
geo_code_He <- geocode("Helsinki")
geo_code_He

##        lon      lat
## 1 24.94102 60.17332

day_length(ymd("2013-09-21"),
           lon = geo_code_He[["lon"]], lat = geo_code_He[["lat"]])

## [1] 12.12728

day_length(ymd("2013-09-21"),
           lon = geo_code_He[["lon"]], lat = geo_code_He[["lat"]],
           twilight = "civil")

## [1] 13.74776

day_length(ymd("2013-09-21"),
           lon = geo_code_He[["lon"]], lat = geo_code_He[["lat"]],
           twilight = "nautical")

## [1] 15.43503

day_length(ymd("2013-09-21"),
           lon = geo_code_He[["lon"]], lat = geo_code_He[["lat"]],
           twilight = "astronomical")

## [1] 17.28531
```

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"),
           lon = geo_code_He[["lon"]], lat = geo_code_He[["lat"]],
           twilight = c(20, 0))

## [1] 9.251774
```

In addition, function `day_night` returns a list containing all the quantities returned by the other functions. As other functions described in this chapter, `day_night` is vectorized for the `date` parameter.

```
day_night(ymd("2013-12-21"),
          lon = geo_code_BA[["lon"]],
          lat = geo_code_BA[["lat"]],
          tz = "America/Argentina/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
```

And with `unit.out` set to `"hour"`

```
day_night(ymd("2013-12-21"),
          lon = geo_code_BA[["lon"]],
          lat = geo_code_BA[["lat"]],
          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
```

13.5 Task: calculating the position of the sun

`sun_angles` not only returns solar elevation, but 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 for the output is by default that currently in use in the computer on which R is

running, but we can easily specify the time coordinates used for the output with parameter `tz`, using any string accepted by package `lubridate`.

```
geo_code_Jo <- geocode("Joensuu")
geo_code_Jo

##        lon      lat
## 1 29.76353 62.60109

my_time <- ymd_hms("2014-05-29 18:00:00", tz="EET")
sun_angles(my_time,
         lon = geo_code_Jo[["lon"]], lat = geo_code_Jo[["lat"]])

## $time
## [1] "2014-05-29 18:00:00 EEST"
##
## $azimuth
## [1] 267.585
##
## $elevation
## [1] 25.81887
##
## $diameter
## [1] 0.5260482
##
## $distance
## [1] 1.013595
```

We can calculate the current position of the sun, in this case giving the position of the sun in the sky of Joensuu when this .PDF file was generated.

```
sun_angles(now(),
         lon = geo_code_Jo[["lon"]], lat = geo_code_Jo[["lat"]])

## $time
## [1] "2015-06-18 18:05:27 EEST"
##
## $azimuth
## [1] 268.9466
##
## $elevation
## [1] 27.12206
##
## $diameter
## [1] 0.5247868
##
## $distance
## [1] 1.016032
```

13.6 Task: plotting sun elevation through a day

Function `sun_angles` described above is vectorized, 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 sun only elevation, plotted for Helsinki through the course of 23 June 2014. We first a vector of times, using `seq` which can not

only be used with numbers, but also with dates. Note that `by` is specified as a string.

```
opts_chunk$set(opts_fig_wide)
```

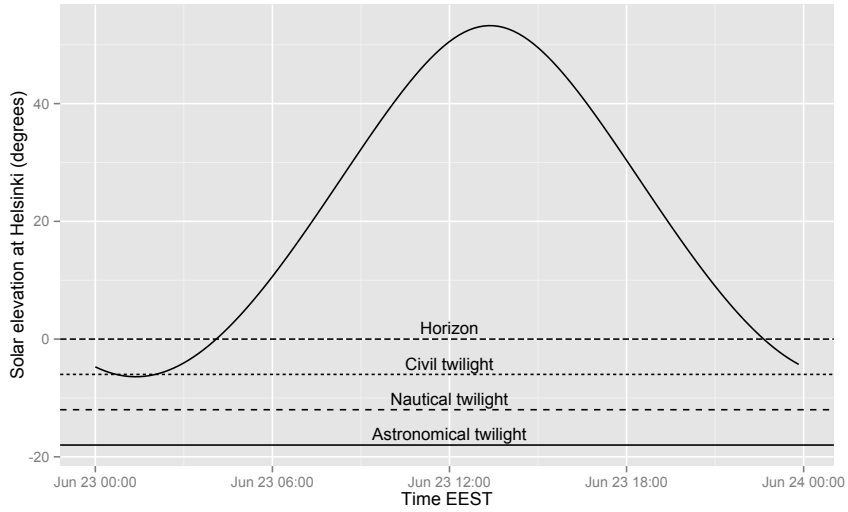
```
hours <- seq(from=ymd("2014-06-23", tz="EET"),
             by="10 min",
             length=24 * 6)
sun_elev_hel <- data.frame(time_eet = hours,
                           elevation =
                             sun_angles(hours,
                                        lon = geo_code_He[["lon"]],
                                        lat = geo_code_He[["lat"]])$elevation,
                           location = "Helsinki",
                           lon = geo_code_He[["lon"]],
                           lat = geo_code_He[["lat"]])
```

We also create a small data frame with data for plotting and labeling the different twilight conventions.

```
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 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")
```



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="3 day")
```

To calculate the length of each day, we need to use an explicit loop as function `day_night` is not vectorized. 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,
                                    lon = geo_code_He[["lon"]],
                                    lat = geo_code_He[["lat"]],
                                    tz = "EET"),
             location = "Helsinki",
             lon = geo_code_He[["lon"]],
             lat = geo_code_He[["lat"]])
```

```
geo_code_Iv <- geocode("Ivalo")
daylengths_ivalo <-
  data.frame(day = days,
             daylength = day_length(days,
                                    lon = geo_code_Iv[["lon"]],
                                    lat = geo_code_Iv[["lat"]],
                                    tz = "EET"),
             location = "Ivalo",
             lon = geo_code_Iv[["lon"]],
```

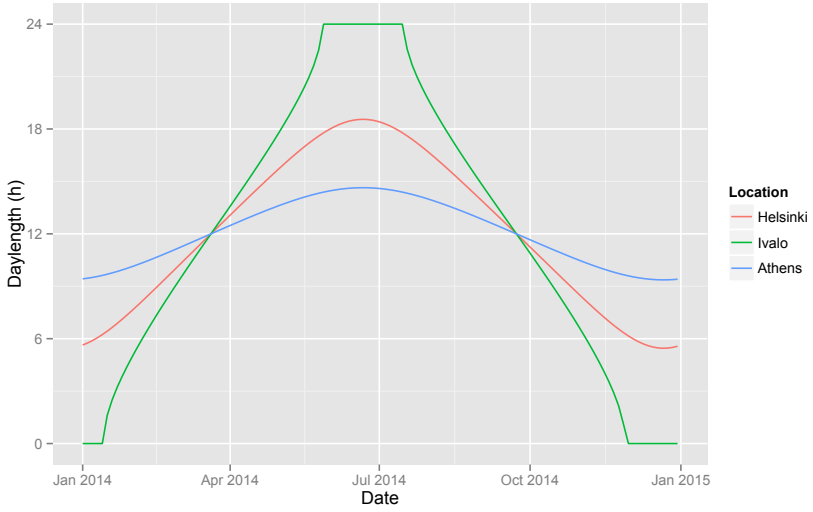
```
              lat = geo_code_Iv[["lat"]])
```

```
geo_code_At <- geocode("Athens, Greece")
daylengths_athens <-
  data.frame(day = days,
             daylength = day_length(days,
                                    lon = geo_code_At[["lon"]],
                                    lat = geo_code_At[["lat"]],
                                    tz = "EET"),
             location = "Athens",
             lon = geo_code_At[["lon"]],
             lat = geo_code_At[["lat"]])
```

```
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,
                                    lon = geo_code_He[["lon"]],
                                    lat = geo_code_He[["lat"]],
                                    tz = "EET", unit.out = "hour"),
             location = "Helsinki",
             lon = geo_code_He[["lon"]],
             lat = geo_code_He[["lat"]])
```

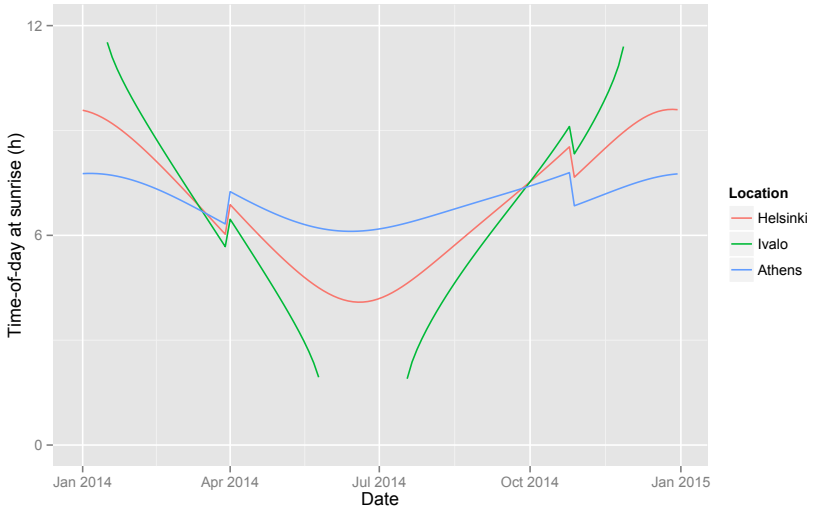
```
geo_code_Iv <- geocode("Ivalo")
sunrise_ivalo <-
  data.frame(day = days,
             sunrise = sunrise_time(days,
                                    lon = geo_code_Iv[["lon"]],
                                    lat = geo_code_Iv[["lat"]],
                                    tz = "EET", unit.out = "hour"),
             location = "Ivalo",
             lon = geo_code_Iv[["lon"]],
             lat = geo_code_Iv[["lat"]])
```

```
geo_code_At <- geocode("Athens, Greece")
sunrise_athens <-
  data.frame(day = days,
             sunrise = sunrise_time(days,
                                    lon = geo_code_At[["lon"]],
                                    lat = geo_code_At[["lat"]],
                                    tz = "EET", unit.out = "hour"),
             location = "Athens",
             lon = geo_code_At[["lon"]],
             lat = geo_code_At[["lat"]])
```

```
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() +
  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 16 rows containing missing values
(geom_path).
```



The breaks in the lines are the result of the changes between winter and summer time coordinates.

```
try(detach(package:photobiology))
try(detach(package:lubridate))
try(detach(package:ggmap))
try(detach(package:ggplot2))
```

CHAPTER 14

Colour

Abstract

In this chapter we explain how to use colours according to visual sensitivity. For example calculating red-green-blue (RGB) values for humans.

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 tri-chromic 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.

> This package is very 'young' so may be to some extent buggy, and/or have rough edges. We plan to add at least visual data for honey bees.

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 `colors`, 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.

## 293-800 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))
```

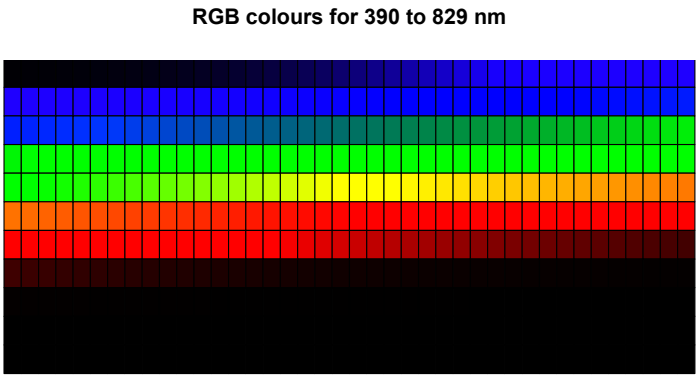
```
## [1] "#59534F"

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))
```

CHAPTER 15

Plotting spectra and colours

Abstract

In this chapter we explain how to plot spectra and colours, using packages `ggplot2`, `ggtern`, and the functions in our package `photobiologygg`. Both `ggtern` for ternary plots and `photobiologygg` for annotating spectra build new functionality on top of the `ggplot2` package. We also use several functions and data from package `photobiology` in the examples.

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(ggplot2)
library(scales)
library(ggtern)

##
## Attaching package:  'ggtern'
##
## The following objects are masked from 'package:ggplot2':
##
##    %+%, %+replace%, aes, calc_element,
##    geom_density2d, geom_segment,
##    geom_smooth, ggplot_build,
##    ggplot_gtable, ggsave, opts,
##    stat_density2d, stat_smooth, theme,
##    theme_bw, theme_classic, theme_get,
##    theme_gray, theme_grey, theme_minimal,
##    theme_set, theme_update

library(gridExtra)
```

```
## Loading required package:  grid

library(photobiology)
library(photobiologyFilters)
library(photobiologyWavebands)
library(photobiologygg)
```

15.2 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 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.

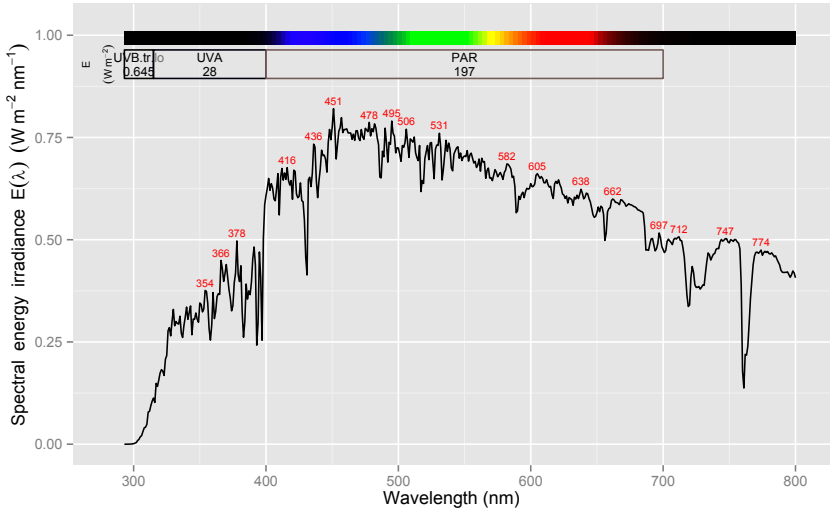
15.3 Task: simple plotting of spectra

Pakage `photobiologygg` defines specializations of the generic `plot` function of R. These functions are available for spectral objects. They return a

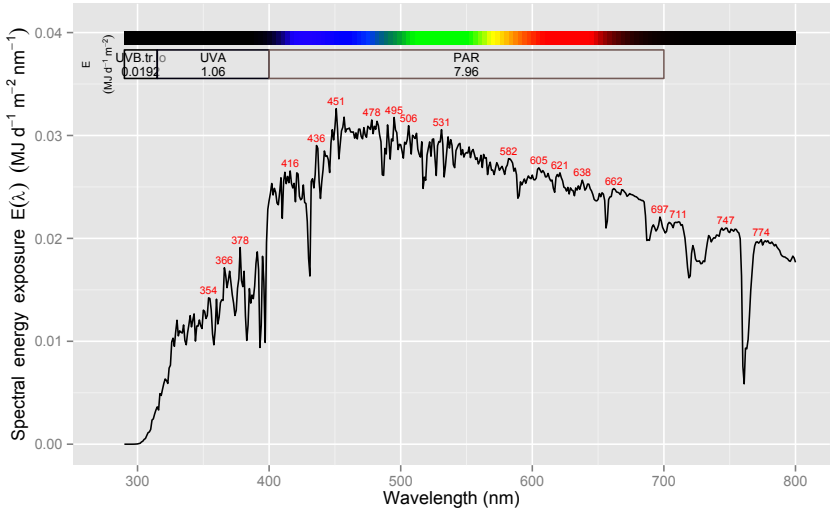
[1] `ggplot2` is feature-frozen, in other words the user interface defined by the functions and their arguments will not change in future versions. Consequently it is a good basis for adding application-specific functionality through separate packages. `ggplot2` uses the *grammar of graphics* for describing 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.

`ggplot` object, to which additional layers can be added if desired. An example of it simplest use follows. As the spectral objects have spectral irradiance expressed in known energy or photon units, and an attribute indicating the time unit, the axis labels are produced automatically. The two plots that follow show spectral irradiance, and spectral daily exposure, respectively.

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

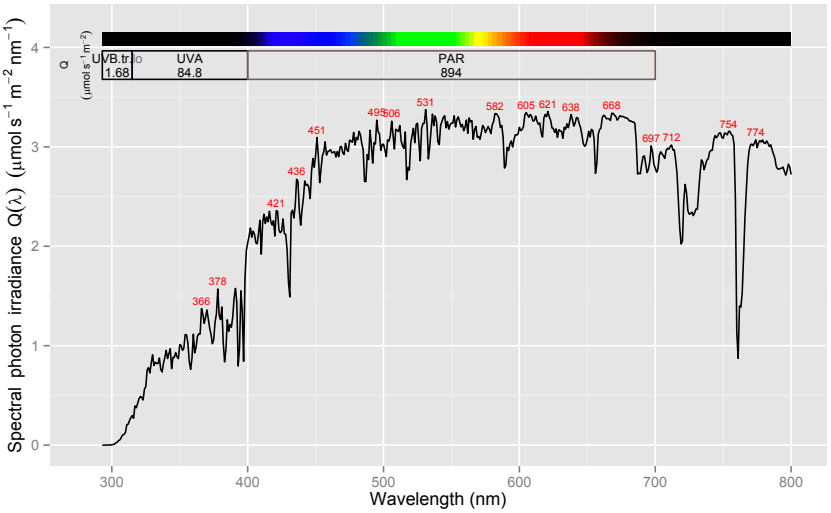



```
plot(sun.daily.spct)
```



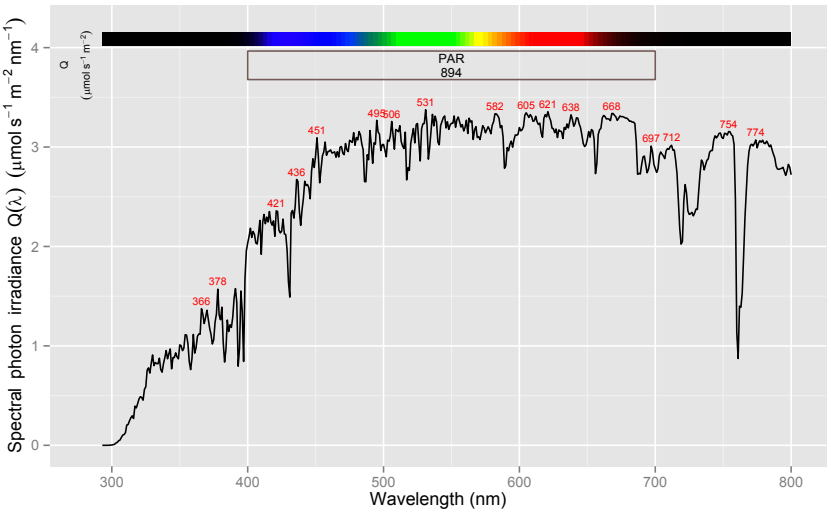
The parameter `unit` can be set to `"photon"` to obtain a plot depicting spectral photon irradiance. This works irrespective of whether the `source_spct` object contains the spectral data in photon or energy units.

```
plot(sun.spct, unit.out = "photon")
```

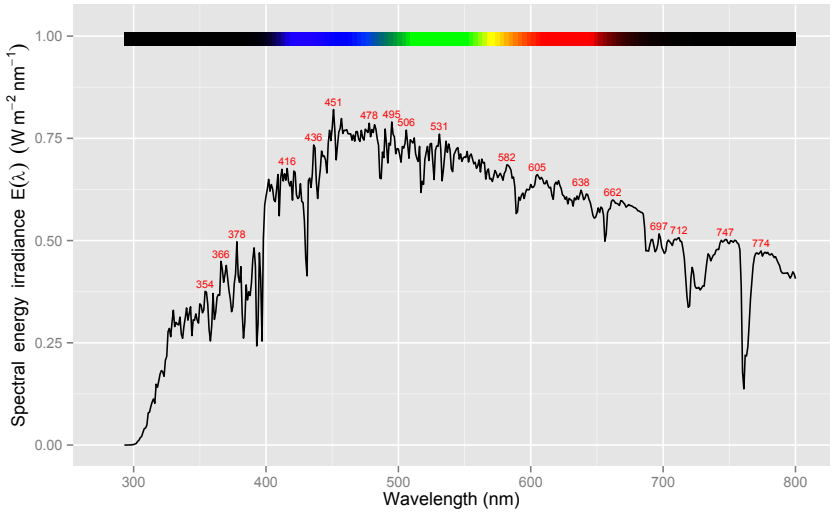


A list of wave bands, or a single wave band, to be used for annotation can be supplied through the `bands` parameter. A `NULL` waveband results in no waveband labels, while the next example shows how to obtain the total irradiance.

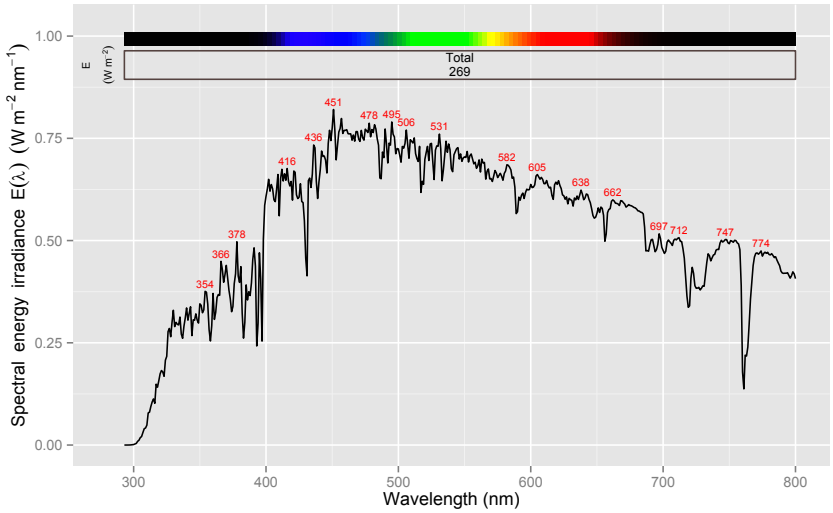
```
plot(sun.spct, w.band = PAR(), unit.out = "photon")
```




```
plot(sun.spct, w.band = NULL)
```

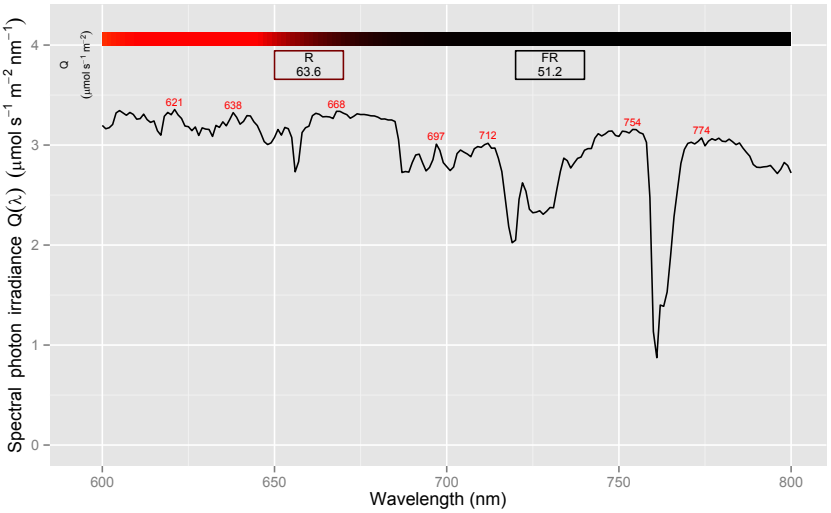



```
plot(sun.spct, w.band = waveband(sun.spct))
```



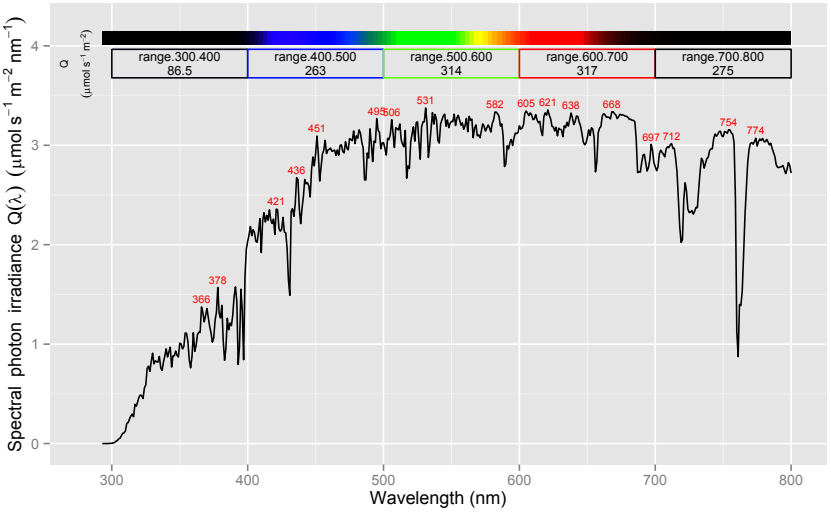
Of course the arguments to these parameters can be supplied in different combinations, and combined with other functions as need. This last example shows how to plot using photon-based units, selecting only a specific region of the spectrum, annotated with the red and far-red photon irradiances, using Prof. Harry Smith's definitions for these two wavebands.

```
plot(trim_spct(sun.spct, waveband(c(600,800))),
     w.band = list(Red("Smith20"), Far_red("Smith20")), unit.out = "photon")
```

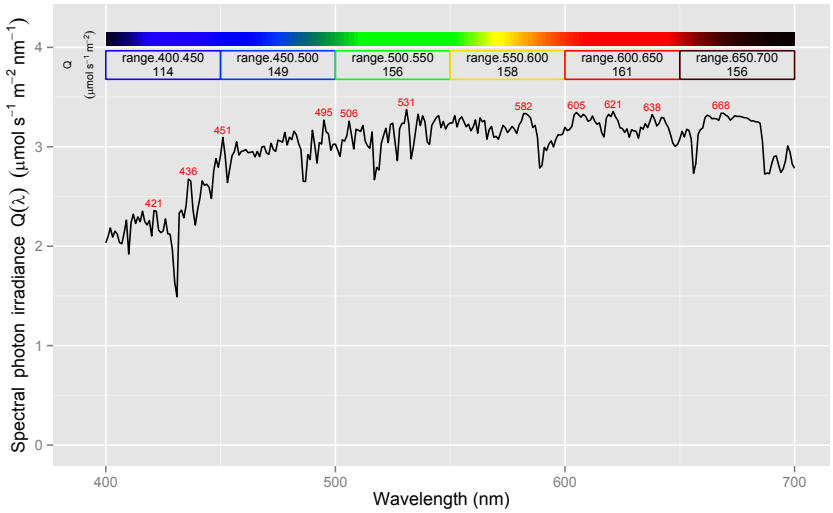


Two final examples show how to annotate a spectrum plot by equal sized wavebands.

```
plot(sun.spct,
     w.band = split_bands(c(300,800), length.out = 5), unit.out = "photon")
```




```
plot(trim_spct(sun.spct, PAR()),
     w.band=split_bands(PAR(), length.out = 6), unit.out = "photon")
```



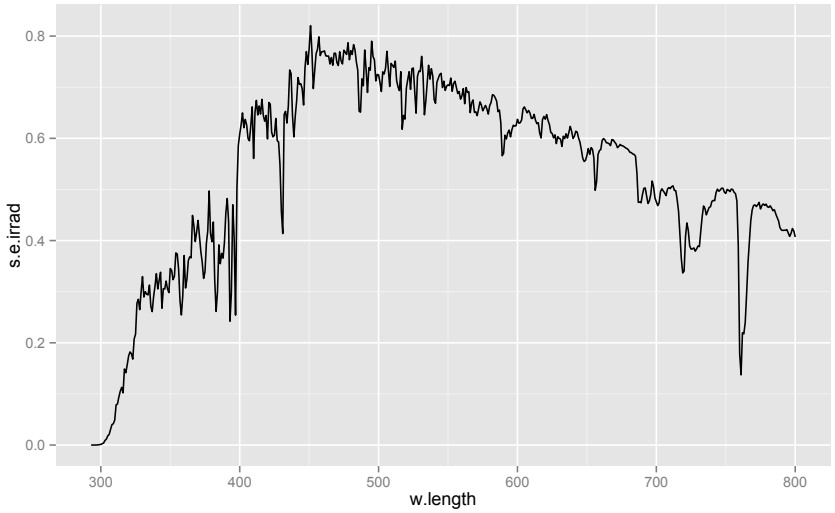
As the current implementation uses annotations rather than a `ggplot` 'statistic', waveband irradiance annotations ignore global aesthetics and facets. If used for simultaneous plotting of several spectra (stored in a single R object), then parameter `w.band` should given `NULL` as argument.

15.4 Task: plotting spectra with `ggplot2`

We create a simple 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.

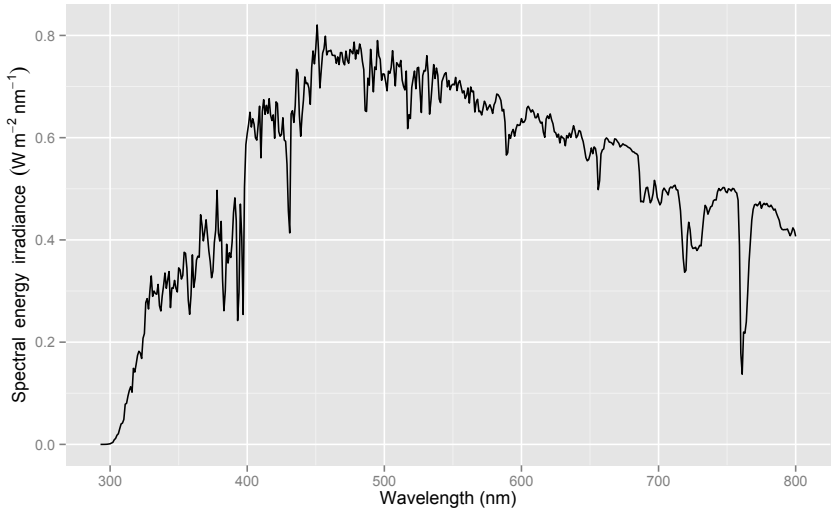
```
fig_sun.e0 <-
  ggplot(data=sun.spct, aes(x=w.length, y=s.e.irrad)) +
  geom_line()

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 `help(plotmath)` and appendix ?? for more details.

```
fig_sun.e0  +
  labs(
    y = expression(Spectral~~energy~~irradiance~~(W~m^{-2}~nm^{-1})),
    x = "Wavelength (nm)")
```



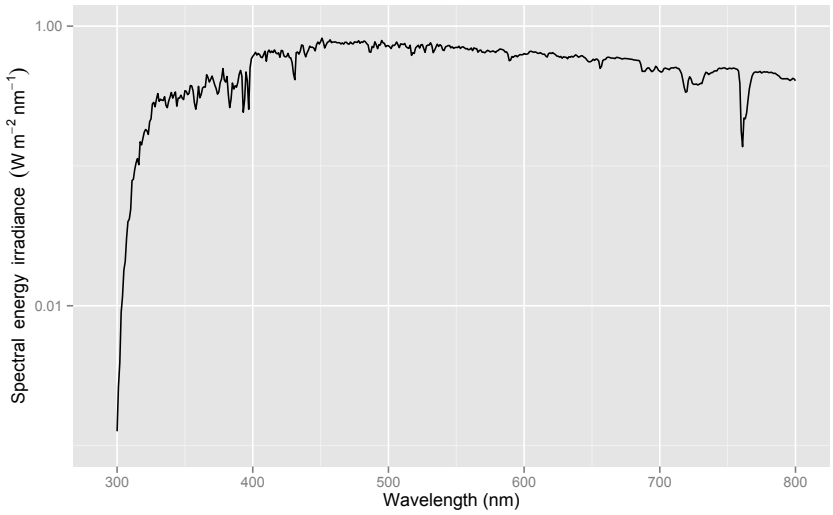
As we are going to re-use the same axis-labels in later plots, it is handy to save their definitions to variables. These definitions will be used in many of this chapter's plots. We also add `atop` to two of the expressions to making shorter versions by setting the spectral irradiance units on a second 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)"
```

15.5 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)

## Warning:  Removed 7 rows containing missing values
(geom_path).
```



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.

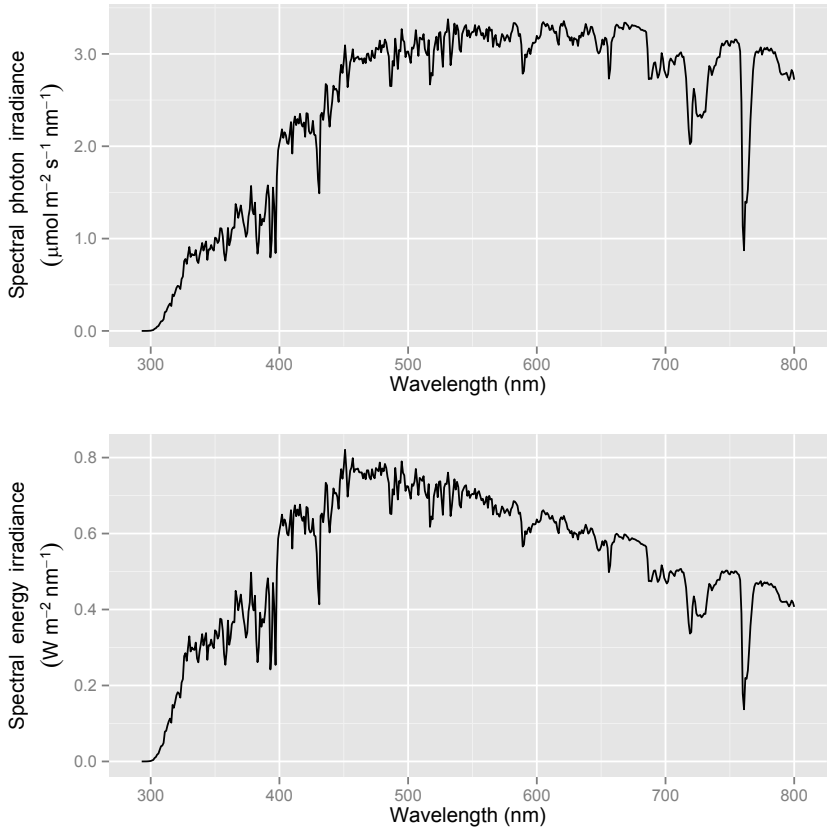
15.6 Task: compare energy and photon spectral units

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.

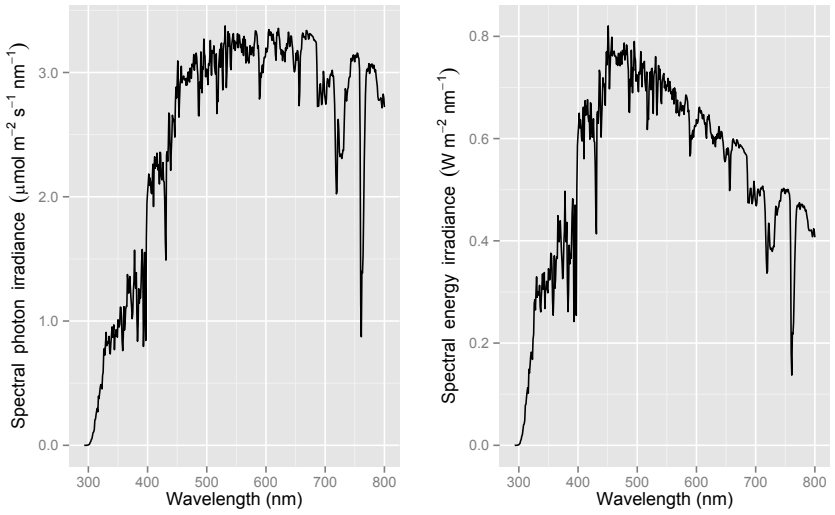
```
num_one_dec <- function(x, ...) {
  format(x, nsmall=1, trim=FALSE, width=4, ...)
  }

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 ggplots, 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)
```



15.7 Task: finding peaks and valleys in spectra

We first show the use of function `get_peaks` that returns the wavelengths at which peaks are located. The parameter `span` determines the number of values used to find a local maximum (the higher the value used, the fewer maxima are detected), and the parameter `ignore_threshold` the fraction of the total span along the irradiance that is taken into account (a value of 0.75, requests only peaks in the upper 25% of the y-range to be returned; a value of -0.75 works similarly but for the lower half of the y-range)[3]. It is good to mention that `head` returns the first six rows of its argument, and we use it here just to reduce the length of the output, if you run these examples yourself, you can remove `head` from the code. In the output, x corresponds to wavelength, and y to spectral irradiance, while `label` is a character string with the wavelength, possibly formatted.

```
head(with(sun.spct,
          get_peaks(w.length, s.e.irrad, span=31)))

##     x         y label
## 1 378 0.4969714   378
## 2 416 0.6761818   416
## 3 451 0.8204633   451
## 4 478 0.7869773   478
## 5 495 0.7899872   495
## 6 531 0.7603297   531

head(with(sun.spct,
          get_peaks(w.length, s.e.irrad, span=31,
                    ignore_threshold=0.75)))

##     x         y label
## 1 416 0.6761818   416
## 2 451 0.8204633   451
## 3 478 0.7869773   478
## 4 495 0.7899872   495
## 5 531 0.7603297   531
## 6 582 0.6853736   582
```

The parameter span, indicates the size in number of observations (e.g. number of discrete wavelength values) included in the window used to find local maxima (peaks) or minima (valleys). By providing different values for this argument we can 'adjust' how *fine* or *coarse* is the structure described by the peaks returned by the function. The window is always defined using an odd number of observations, if an even number is provided as argument, it is increased by one, with a warning.

```
head(with(sun.spct,
          get_peaks(w.length, s.e.irrad, span=21)))

##     x         y label
```

[3] In the current example setting `ignore_threshold` equal to 0.75 given that the range of the spectral irradiance data goes from 0.00 $\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}$ to 0.82 $\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}$, causes any peaks having a spectral irradiance of less than 0.62 $\mu mol\,m^{-2}\,s^{-1}\,nm^{-1}$ to be ignored.

```
## 1 354 0.3758625   354
## 2 366 0.4491898   366
## 3 378 0.4969714   378
## 4 416 0.6761818   416
## 5 436 0.7336607   436
## 6 451 0.8204633   451

head(with(sun.spct,
          get_peaks(w.length, s.e.irrad, span=51)))

##     x         y label
## 1 451 0.8204633   451
## 2 495 0.7899872   495
## 3 747 0.5025733   747
```

The equivalent function for finding valleys is `get_valleys` taking the same parameters as `get_peaks` but returning the wavelengths at which the valleys are located.

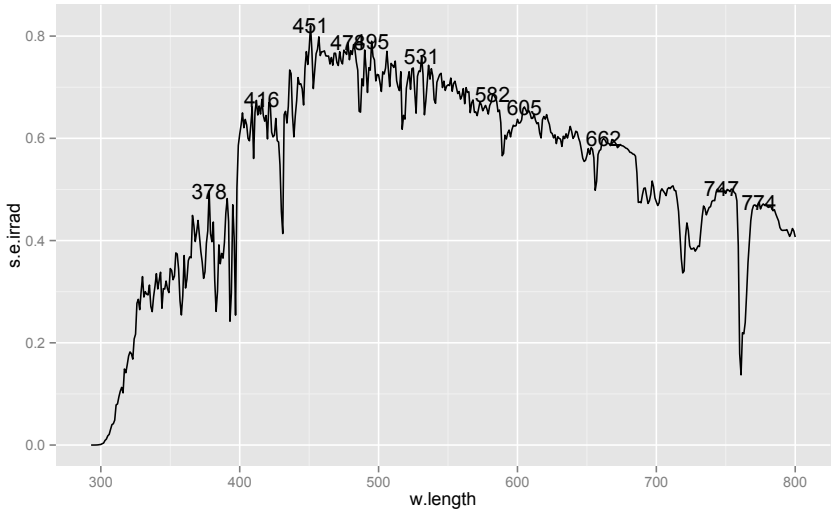
```
head(with(sun.spct,
          get_valleys(w.length, s.e.irrad, span=51)))

##     x         y label
## 1 358 0.2544907   358
## 2 393 0.2422023   393
## 3 431 0.4136900   431
## 4 487 0.6511654   487
## 5 517 0.6176652   517
## 6 589 0.5658760   589

head(with(sun.spct,
          get_valleys(w.length, s.e.irrad, span=51,
                      ignore_threshold=0.5)))

##     x         y label
## 1 431 0.4136900   431
## 2 487 0.6511654   487
## 3 517 0.6176652   517
## 4 589 0.5658760   589
## 5 656 0.4982959   656
```

In the next section, we plot spectra and annotate them with peaks and valleys. If you find the meaning of the parameters `span` and `ignore_threshold` difficult to grasp from the explanation given above, please, study the code and plots in section 15.8.

15.8 Task: annotating peaks and valleys in spectra

Here we show an example of the use the new `ggplot` 'statistics' `stat_peaks` from our package `photobiologygg`. It uses the same parameter names and take the same arguments as the `get_peaks` function described in section 15.7. We reuse once more `fig_sun.e` saved in section 15.4.

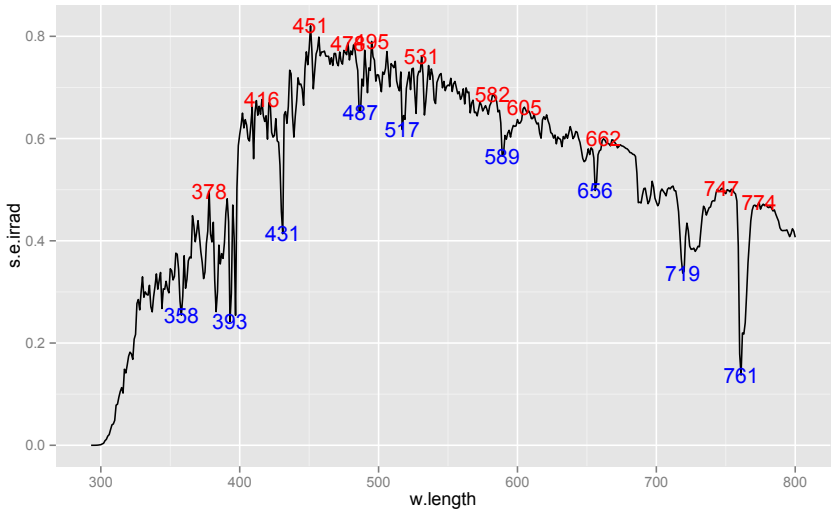
```
fig_sun.e0 + stat_peaks(span=31)
```



Now we play with `ggplot2` to show different ways of plotting the peaks and valleys. It behaves as a `ggplot2` `stat_xxxx` function accepting a `geom` argument and all the aesthetics valid for the chosen geom. By default `geom_text` is used.

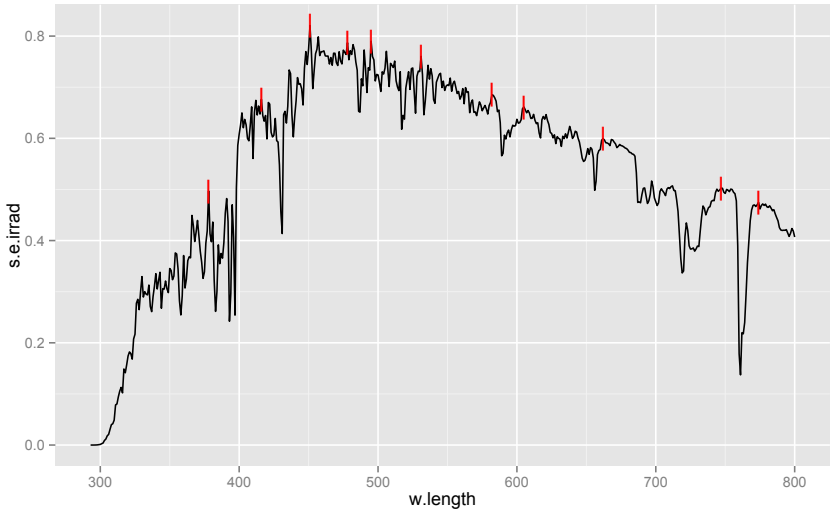
We can change aesthetics, for example the colour:

```
fig_sun.e0 + stat_peaks(colour="red", span=31) +
             stat_valleys(colour="blue", span=51)
```



We can also use a different geom, in this case `geom_point`, however, be aware that the `geom` parameter takes as argument a character string giving the name of the geom, in this case `"point"`. We change a few additional aesthetics of the points: we set `shape` to a character, and set its size to 6.

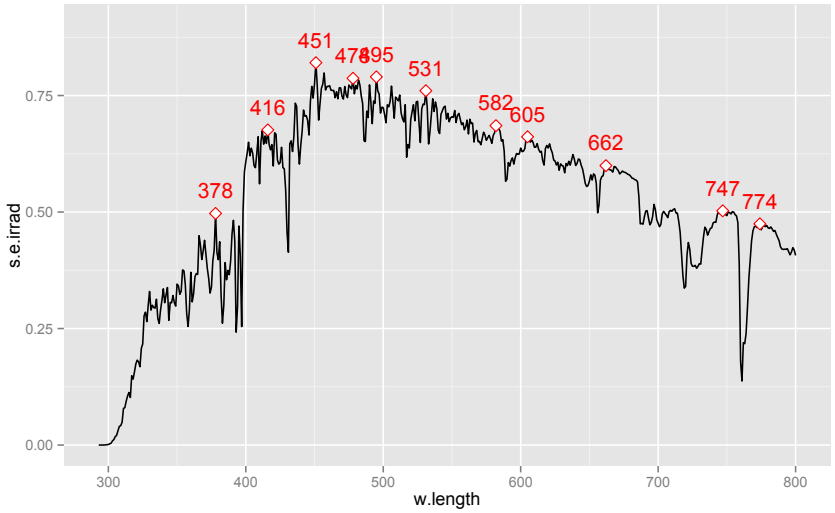
```
fig_sun.e0 +
  stat_peaks(colour="red", geom="point",
             shape="|", size=6, span=31)
```



We can add the same `stat` two or more times to a ggplot, 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[4] In addition we expand the y-axis scale so that all labels fall within the plotting area.

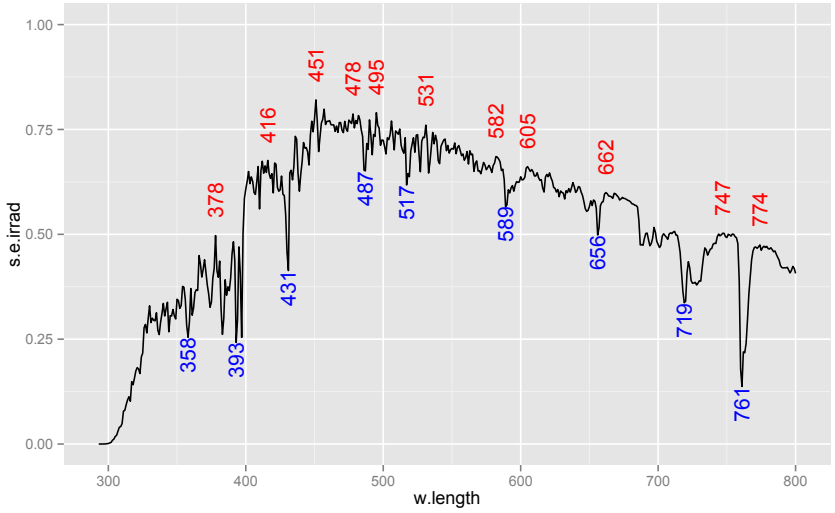
```
fig_sun.e0 +
  stat_peaks(colour="red", geom="point", shape=23,
             fill="white", size=3, span=31) +
  stat_peaks(colour="red", vjust=-1, span=31) +
  expand_limits(y=0.9)
```

[4]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.



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.

```
fig_sun.e0 +
  stat_peaks(angle=90, hjust=-0.5, colour="red", span=31) +
  stat_valleys(angle=90, hjust=1, color="blue", span=51) +
  expand_limits(y=1.0)
```



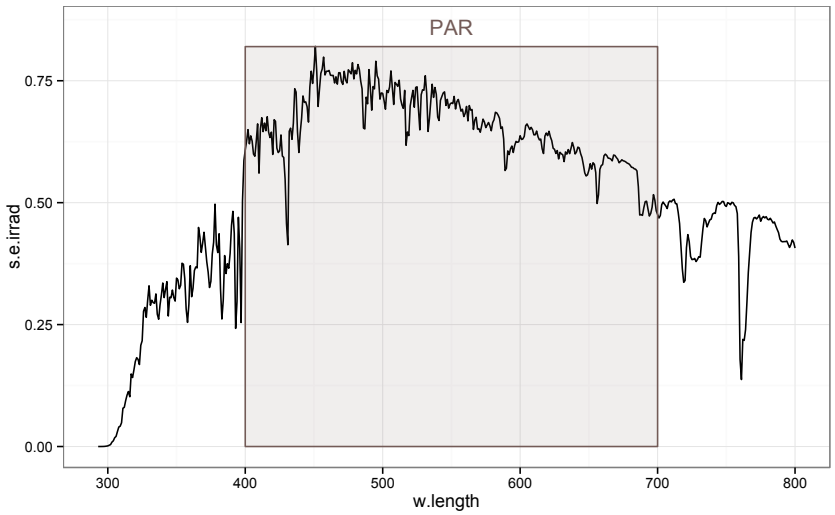
See section ?? in chapter ?? for an example these stats together with facets.

15.9 Task: annotating wavebands

The function `annotate_waveband` can be used to highlight a waveband in a plot of spectral data. Its first argument should be a `waveband` object, and the second argument a `geom` as a character string. The positions on the x-axis are calculated automatically by default, but they can be overridden by explicit arguments. The vertical positions have no default, except for `ymin` which is equal to zero by default. The colour has a default value calculated from waveband definition, in addition x is by default set to the midpoint of the waveband along the wavelength limits. The default value of the labels is the 'name' of the waveband as returned by `labels.waveband`.

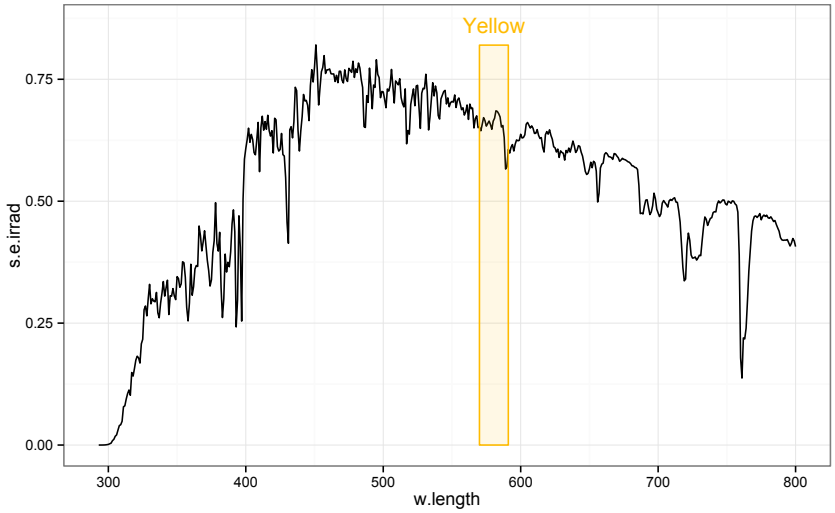
Here is an example for PAR using defaults, and with arguments supplied only for parameters with no defaults. The example does the annotation using two different 'geoms', `"rect"` for marking the region, and `"text"` for the labels.

```
figvl <- fig_sun.e0 + annotate_waveband(PAR(), "rect", ymax=0.82) +
                      annotate_waveband(PAR(), "text", y=0.86)

figvl + theme_bw()
```



This example annotates a narrow waveband.

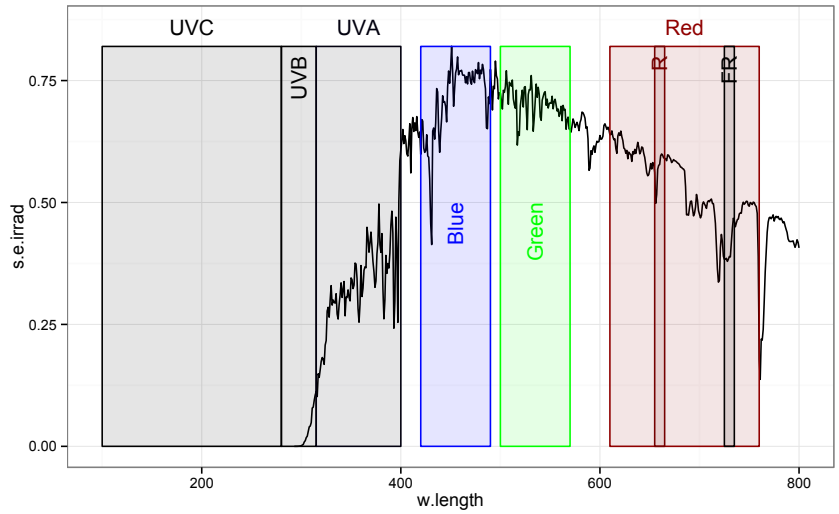
```
figvl <- fig_sun.e0 + annotate_waveband(Yellow(), "rect", ymax=0.82) +
                      annotate_waveband(Yellow(), "text", y=0.86)

figvl + theme_bw()
```



Now an example that is more complex, and demonstrates the flexibility of plots produced with `ggplot2`. We add annotations for eight different wavebands, some of them overlapping. For each one we use two 'geoms' and some labels are rotated and justified. We can also see in this example that the annotations look nicer on a white background, which can be obtained with `theme_bw`. A much simpler, but less flexible approach for adding annotations for several wavebands is described on page 182.

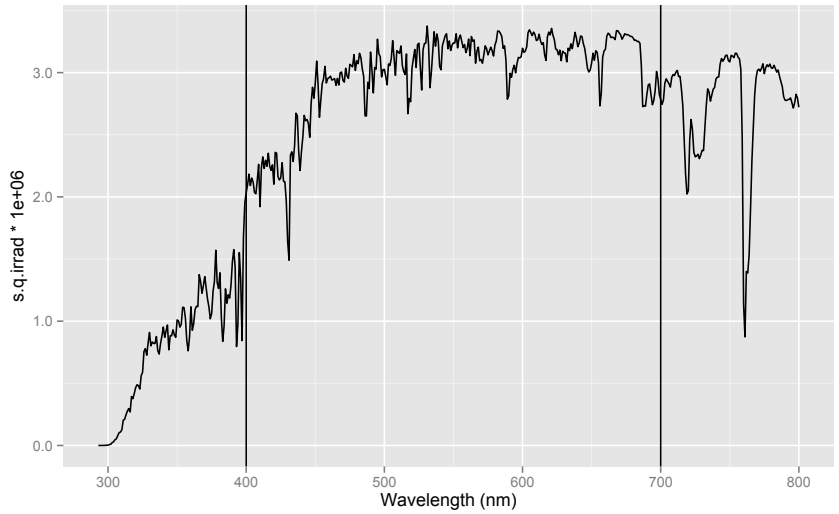
```
figv2 <- fig_sun.e0 +
  annotate_waveband(UVC(), "rect",
                    ymax=0.82) +
  annotate_waveband(UVC(), "text",
                    y=0.86) +
  annotate_waveband(UVB(), "rect",
                    ymax=0.82) +
  annotate_waveband(UVB(), "text",
                    y=0.80, angle=90, hjust=1) +
  annotate_waveband(UVA(), "rect",
                    ymax=0.82) +
  annotate_waveband(UVA(), "text",
                    y=0.86) +
  annotate_waveband(Blue("Sellaro"), "rect",
                    ymax=0.82) +
  annotate_waveband(Blue("Sellaro"), "text",
                    y=0.5, angle=90, hjust=1) +
  annotate_waveband(Green("Sellaro"), "rect",
                    ymax=0.82) +
  annotate_waveband(Green("Sellaro"), "text",
                    y=0.50, angle=90, hjust=1) +
  annotate_waveband(Red(), "rect",
                    ymax=0.82) +
  annotate_waveband(Red(), "text",
                    y=0.86) +
  annotate_waveband(Red("Smith10"), "rect",
                    ymax=0.82) +
  annotate_waveband(Red("Smith10"), "text",
                    y=0.80, angle=90, hjust=1) +
```

```
  annotate_waveband(Far_red("Smith10"), "rect",
                    ymax=0.82) +
  annotate_waveband(Far_red("Smith10"), "text",
                    y=0.80, angle=90, hjust=1)

figv2 + theme_bw()
```



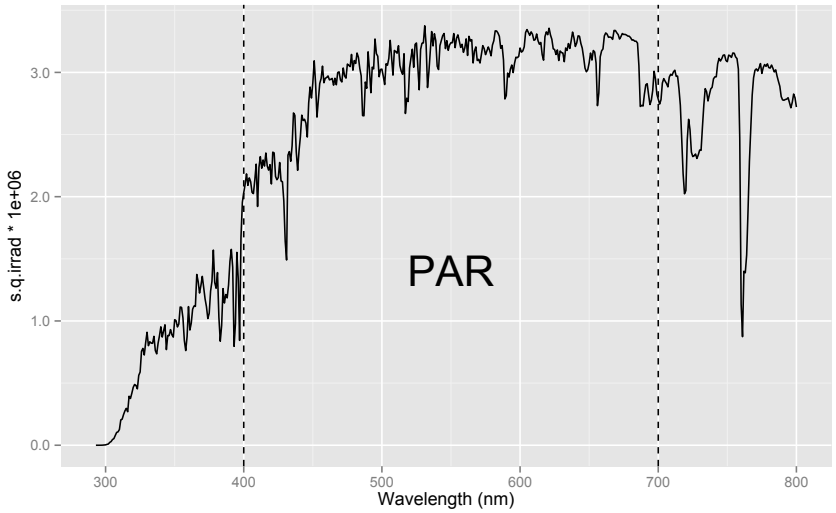
A simple example using `geom_vline`:

```
figvl3 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()))

figvl3
```



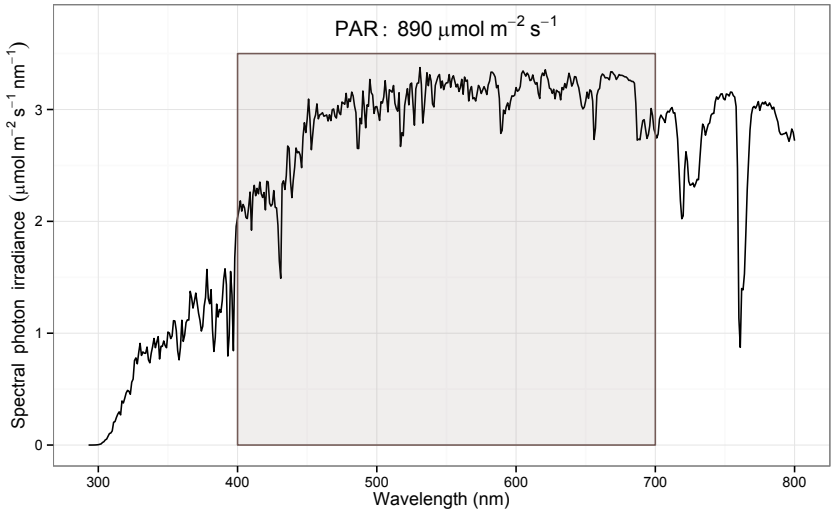
And one where we change some of the aesthetics, and add a label:

```
figvl4 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()), linetype="dashed") +
  annotate_waveband(PAR(), "text", y=1.4, size=10, colour="black")

figvl4
```



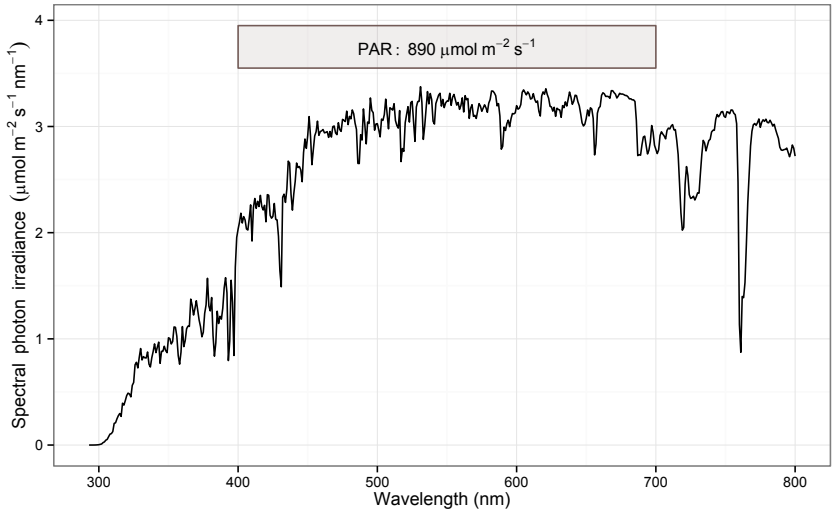
Now including calculated values in the label, first with a simple example with only PAR. Because of using expressions to obtain superscripts we need to add `parse=TRUE` to the call. In addition as we are expressing the integral in photon based units, we also change the type of units used for plotting 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`.

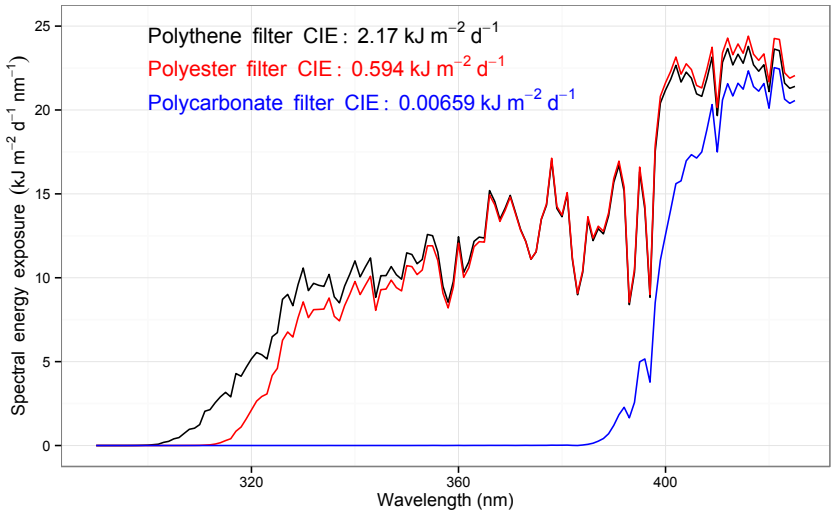
```
fig_sun <- ggplot(data=sun.spct,
                  aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  labs(y = ylab_umol,
       x = "Wavelength (nm)")

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 * polythene.new.spct,
         aes(x=w.length, y=s.e.irrad * 1e-3)) + geom_line() +
  geom_line(data=sun.daily.spct * polyester.new.spct,
            colour="red") +
  geom_line(data=sun.daily.spct * PC.spct,
            colour="blue") +
  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.new.spct, CIE()) * 1e-3
cie.ps <-
  e_irrad(sun.daily.spct * polyester.new.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()
```



15.10 Task: 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 15.10.2 we show code based on tagging spectral data, and in section 15.10.3 the case of using different data for plotting the guide or key is described.

15.10.1 Scale definitions

First we define some new scales for use for plotting with `ggplot` when plotting wavelength derived colours. In the future something equivalent may be included in package `photobiologygg` as predefined scales. We define two very similar scales, one for colour, and one for fill aesthetics.

```
scale_colour_tgspct <-
  function(...,
           tg.spct,
           labels = NULL,
```

```
            guide = NULL,
            na.value=NA) {
    spct.tags <- attr(tg.spct, "spct.tags", exact=TRUE)
    if (is.null(guide)){
      if (spct.tags$wb.num > 12) {
        guide = "none"
      } else {
        guide = guide_legend(title=NULL)
      }
    }
    values <- as.character(spct.tags$wb.colors)
    if (is.null(labels)) {
      labels <- spct.tags$wb.names
    }
    ggplot2:::manual_scale("colour",
                           values = values,
                           labels = labels,
                           guide = guide,
                           na.value = na.value,
                           ...)
}
```

```
scale_fill_tgspct <-
  function(...,
           tg.spct,
           labels = NULL,
           guide = NULL,
           na.value=NA) {
    spct.tags <- attr(tg.spct, "spct.tags", exact=TRUE)
    if (is.null(guide)){
      if (spct.tags$wb.num > 12) {
        guide = "none"
      } else {
        guide = guide_legend(title=NULL)
      }
    }
    values <- as.character(spct.tags$wb.colors)
    if (is.null(labels)) {
      labels <- spct.tags$wb.names
    }

    ggplot2:::manual_scale("fill",
                           values = values,
                           labels = labels,
                           guide = guide,
                           na.value = na.value,
                           ...)
}
```

15.10.2 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 <- copy(sun.spct)
tag(cp.sun.spct)

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
## 507:      799 4.185850e-01 2.795738e-06  #000000
## 508:      800 4.069055e-01 2.721132e-06  #000000
##       wb.f
##    1:   NA
##    2:   NA
##   ---
## 507:   NA
## 508:   NA
```

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 <- copy(sun.spct)
tag(uvb.sun.spct, UVB())

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
## 508:      799 4.185850e-01 2.795738e-06  #000000
## 509:      800 4.069055e-01 2.721132e-06  #000000
##            wb.f
##    1: UVB.tr.lo
##    2: UVB.tr.lo
##   ---
## 508:        NA
## 509:        NA

levels(uvb.sun.spct[["wb.f"]])

## [1] "UVB.tr.lo"
```

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.

```
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

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
```

```
## 508:       799 4.185850e-01 2.795738e-06  #000000
## 509:       800 4.069055e-01 2.721132e-06  #000000
##            wb.f
##   1: UVB.tr.lo
##   2: UVB.tr.lo
##  ---
## 508:         NA
## 509:         NA

levels(uvb.sun.spct[["wb.f"]])

## [1] "UVB.tr.lo"
```

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 <- copy(sun.spct)
tag(plant.sun.spct, Plant_bands())

##      w.length    s.e.irrad    s.q.irrad wl.color
##   1:       293 2.609665e-06 6.391730e-12  #000000
##   2:       294 6.142401e-06 1.509564e-11  #000000
##  ---
## 517:       799 4.185850e-01 2.795738e-06  #000000
## 518:       800 4.069055e-01 2.721132e-06  #000000
##            wb.f
##   1: UVB.tr.lo
##   2: UVB.tr.lo
##  ---
## 517:         NA
## 518:         NA

levels(plant.sun.spct[["wb.f"]])

## [1] "UVB.tr.lo" "UVA"       "Blue"
## [4] "Green"     "R"         "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] 0
##
## $wb.colors
## [1] NA
##
## $wb.names
## [1] NA
##
## $wb.list
## NULL

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
## $wb.colors[[1]]
## [1] "black"
##
##
## $wb.names
## [1] "UVB.tr.lo"
##
## $wb.list
## $wb.list[[1]]
## UVB.ISO.tr.lo
## low (nm) 293
## high (nm) 315
## weighted none
```

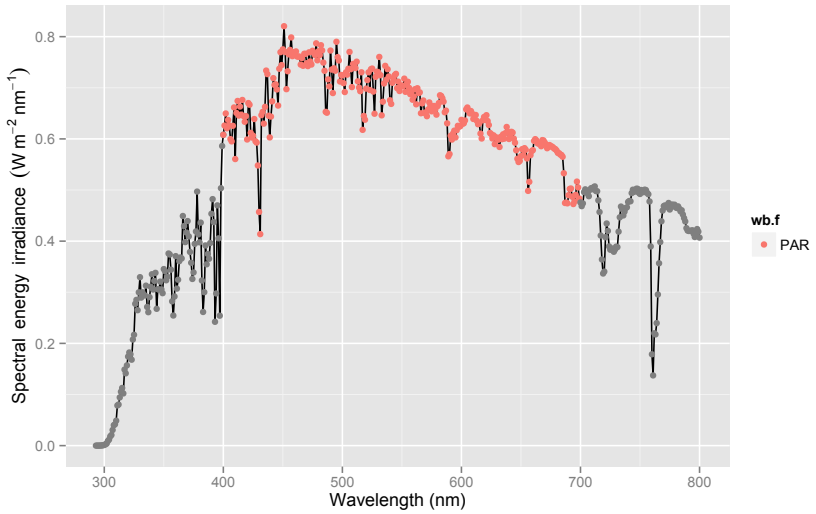
We now tag a spectrum for use in our first plot example.

```
par.sun.spct <- copy(sun.spct)
tag(par.sun.spct, PAR())

##      w.length    s.e.irrad    s.q.irrad wl.color
##   1:      293 2.609665e-06 6.391730e-12  #000000
##   2:      294 6.142401e-06 1.509564e-11  #000000
##  ---
## 509:      799 4.185850e-01 2.795738e-06  #000000
## 510:      800 4.069055e-01 2.721132e-06  #000000
##      wb.f
##   1:   NA
##   2:   NA
##  ---
```

```
## 509:    NA
## 510:    NA
```

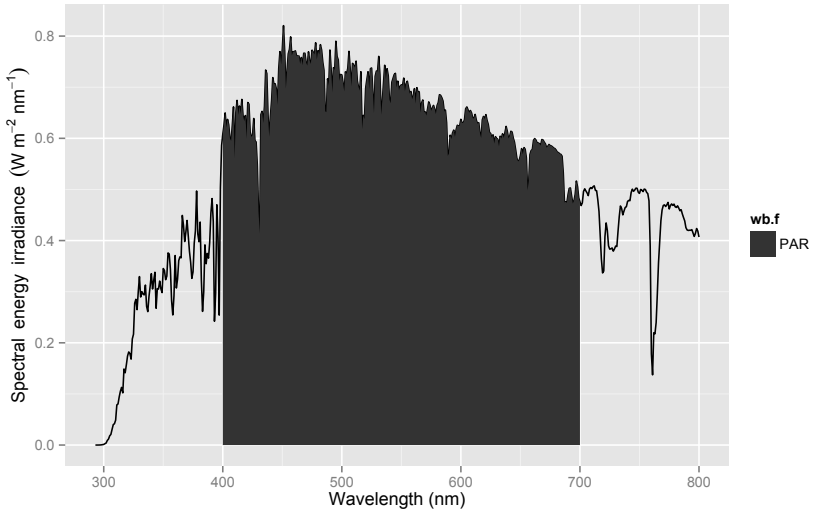
Here we simply use the `wb.f` factor that was added as part of the tagging, with the default colour scale of `ggplot2`, which results in a palette unrelated to the real colour of the different wavelengths.

```
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
```



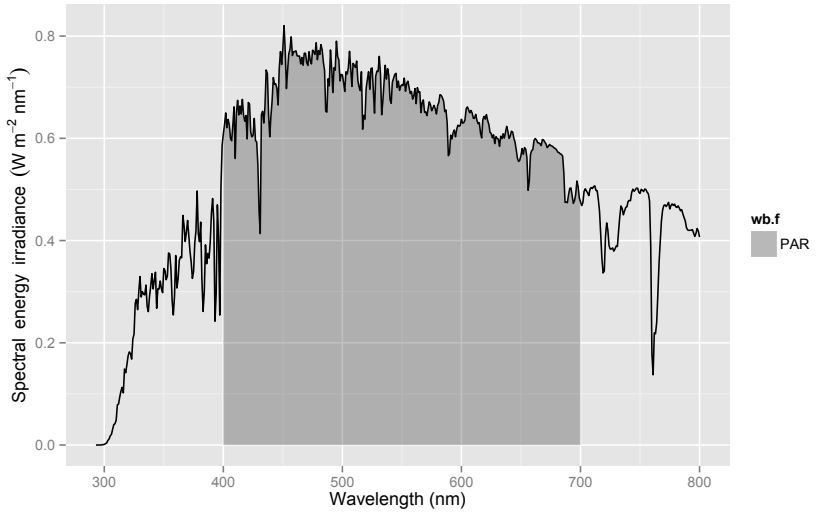
We can also use other geoms like `geom_area` in the next chunk, together with, as an example, a grey fill scale from `ggplot2`.

```
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[5]. We tag each observation in the solar spectrum with human vision colours as defined by ISO.

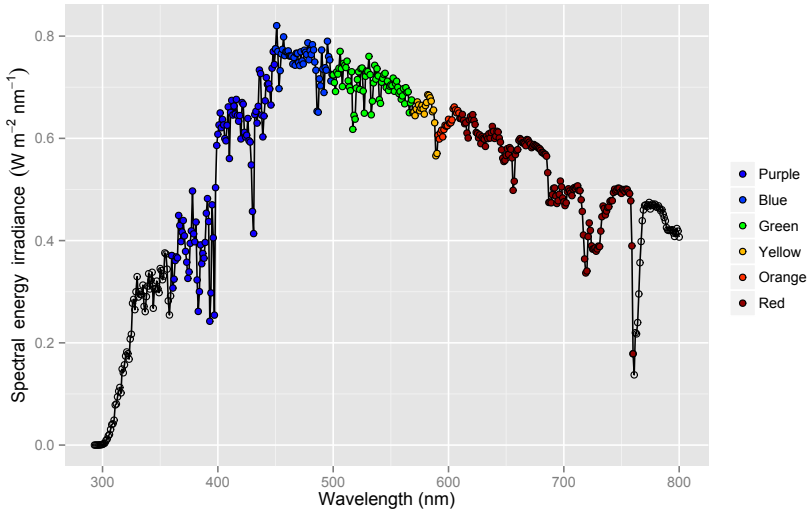
```
tg.sun.spct <- copy(sun.spct)
tag(tg.sun.spct, VIS_bands())

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
## 514:      799 4.185850e-01 2.795738e-06  #000000
## 515:      800 4.069055e-01 2.721132e-06  #000000
##       wb.f
##    1:   NA
##    2:   NA
##   ---
## 514:   NA
## 515:   NA
```

See section 15.10.1 on page 159 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 so those points are not filled. One can play with the `size` of points until ones get the result wanted. The default 'shape' used by `ggplot2` do not accept a `fill` aesthetic, while shape '21' gives circles that can be 'filled'.

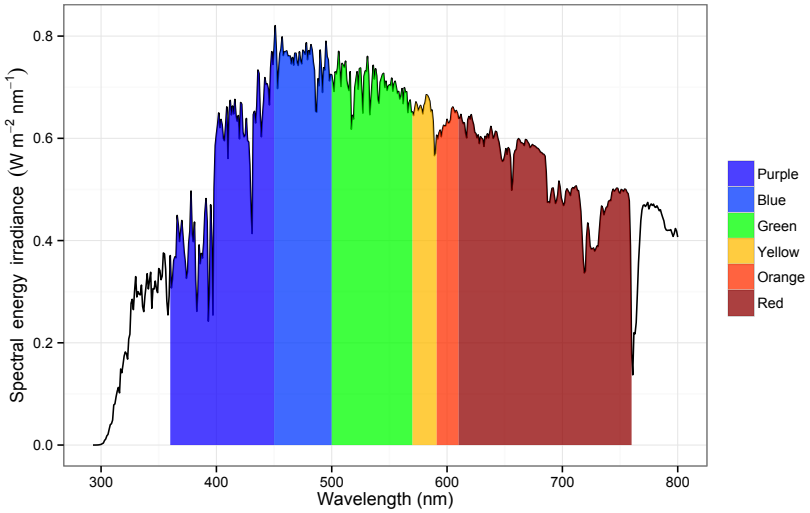
[5]We may want to increase the number of 'observations' in the spectrum by interpolation if there are too few observations for a smooth colour gradient.

```
fig_sun.t02 <-
  ggplot(data=tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  scale_fill_tgspct(tg.spct=tg.sun.spct) +
  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 NAs 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_tgspct(tg.spct=tg.sun.spct) +
  geom_line() +
  geom_area(aes(fill=wb.f), alpha=0.75) +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.t03 + theme_bw()
```

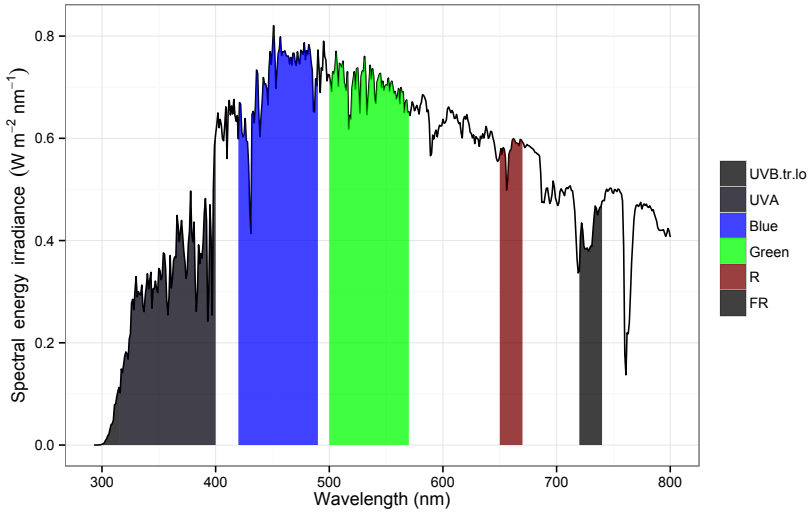


In the next example we tag the solar spectrum with colours using the definitions of plant sensory 'colours'.

```
pl.sun.spct <- copy(sun.spct)
tag(pl.sun.spct, Plant_bands())

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
## 517:      799 4.185850e-01 2.795738e-06  #000000
## 518:      800 4.069055e-01 2.721132e-06  #000000
##           wb.f
##    1: UVB.tr.lo
##    2: UVB.tr.lo
##   ---
## 517:        NA
## 518:        NA
```

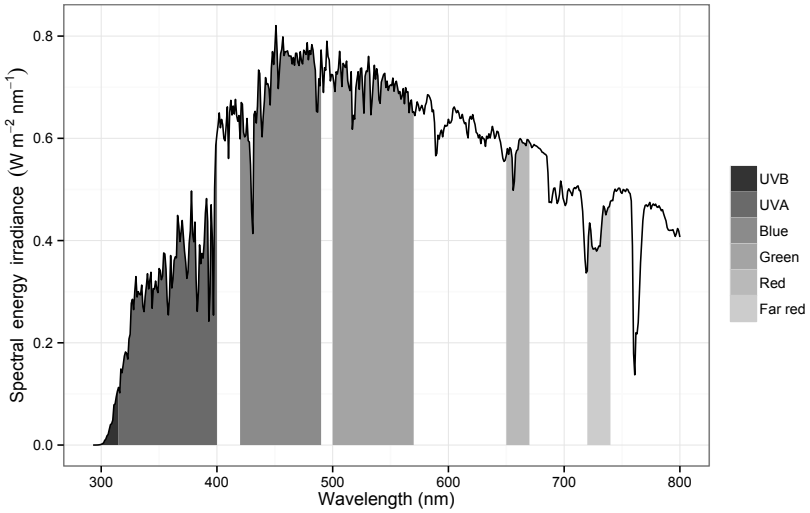
Here we plot the wavebands corresponding to plant sensory 'colours', using the spectrum we tagged in the previous code chunk.

```
fig_sun.pl0 <-
  ggplot(pl.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_tgspct(tg.spct=pl.sun.spct) +
  geom_line() +
  geom_area(aes(fill=wb.f), 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.

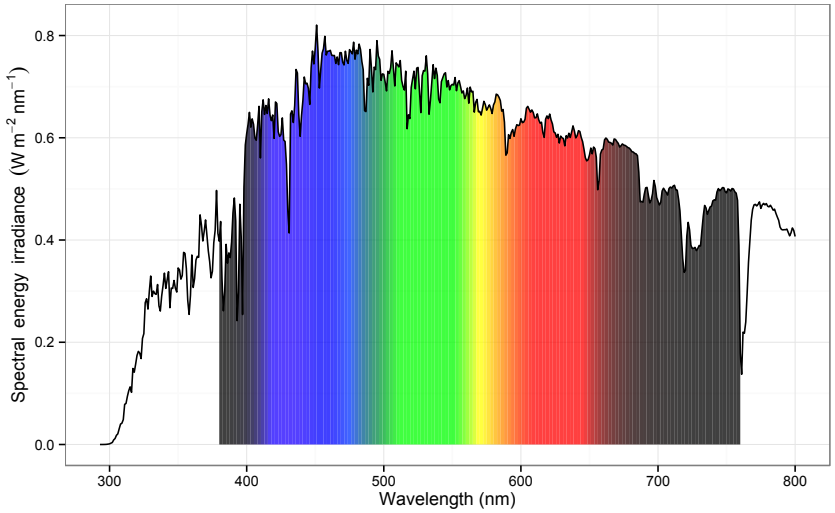
```
interpolate_spct(sun.spct, length.out=800)
```

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 <- copy(sun.spct)
tag(splt.sun.spct, split_bands(VIS(), length.out=150))

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1:      293 2.609665e-06 6.391730e-12  #000000
##    2:      294 6.142401e-06 1.509564e-11  #000000
##   ---
## 798:      799 4.185850e-01 2.795738e-06  #000000
## 799:      800 4.069055e-01 2.721132e-06  #000000
##       wb.f
##    1:   NA
##    2:   NA
##   ---
## 798:   NA
## 799:   NA
```

In the code above, we made a copy of `sun.spct` because being part of the package, it is write protected, and `tag` works by modifying its argument.

```
fig_sun.splt0 <-
  ggplot(splt.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_tgspct(tg.spct=splt.sun.spct) +
  geom_area(aes(fill=wb.f), alpha=0.75) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.splt0 + theme_bw()
```

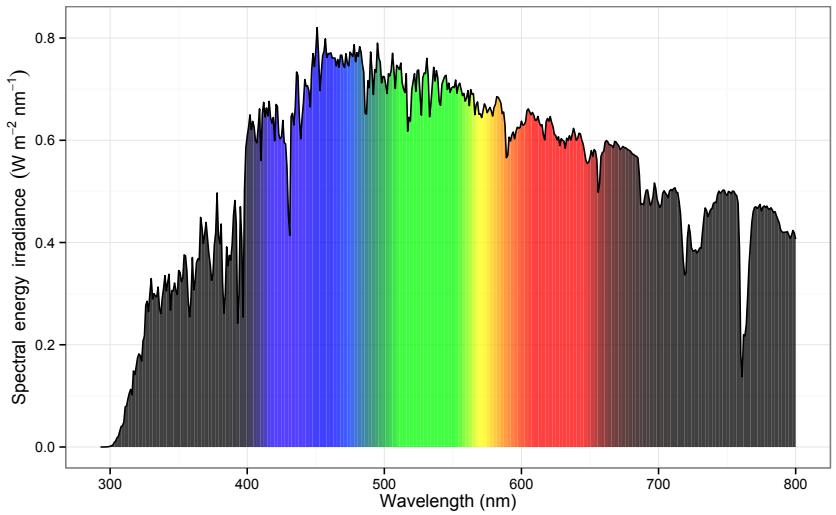


In this other example we tag the whole spectrum, dividing it into 200 wavebands.

```
splt1.sun.spct <- copy(sun.spct)
# splt1.sun.spct <- interpolate_spct(splt1.sun.spct, length.out=1000)
tag(splt1.sun.spct, split_bands(sun.spct, length.out=200))

##       w.length    s.e.irrad    s.q.irrad wl.color
##    1: 293.0000 2.609665e-06 6.391730e-12  #000000
##    2: 294.0000 6.142401e-06 1.509564e-11  #000000
##   ---
## 906: 799.9999 4.069067e-01 2.721139e-06  #000000
## 907: 800.0000 4.069055e-01 2.721132e-06  #000000
##        wb.f
##    1:   wb1
##    2:   wb1
##   ---
## 906: wb200
## 907:    NA
```

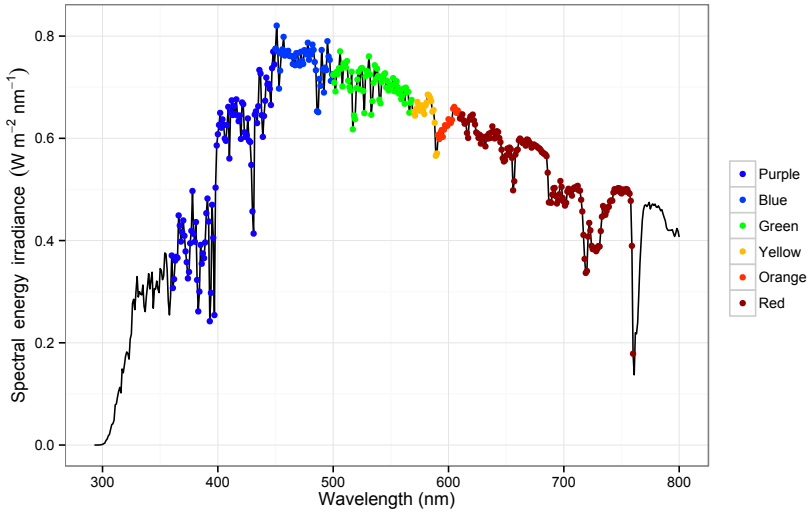
We use `geom_area` and `fill`, and colour the area under the curve. This does not work with `geom_line` because there would not be anything to fill, here we use `geom_area` instead.

```
fig_sun.splt1 <-
  ggplot(splt1.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_fill_tgspct(tg.spct=splt1.sun.spct) +
  geom_area(aes(fill=wb.f), alpha=0.75) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.splt1 + theme_bw()
```



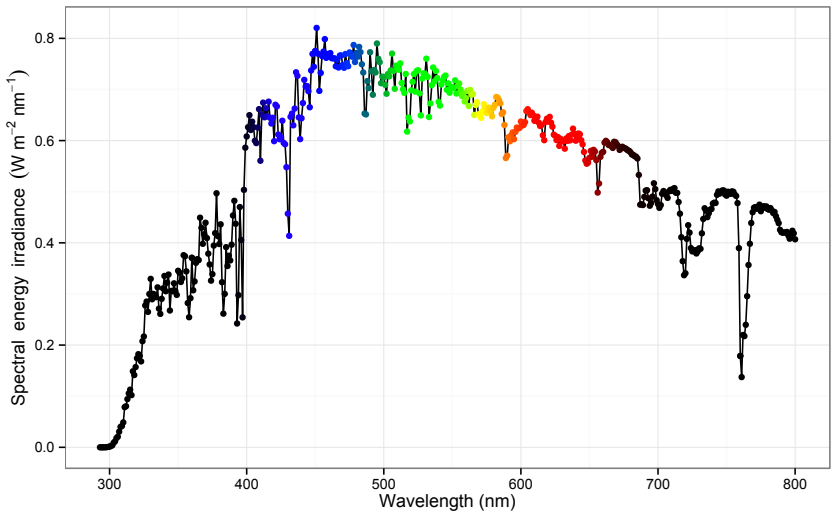
The next example uses `geom_point` and `colour` to color the data points according the waveband they are included in.

```
fig_sun.tg1 <-
  ggplot(tg.sun.spct,
         aes(x=w.length, y=s.e.irrad)) +
  scale_colour_tgspct(tg.spct=tg.sun.spct) +
  geom_line() +
  geom_point(aes(colour=wb.f)) +
  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.

15.10.3 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 geoms. 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 predefined 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())

##    w.length s.e.irrad s.q.irrad Tfr Rfl
## 1: 399.9999         0         0   0   0
## 2: 400.0000         0         0   0   0
## 3: 699.9999         0         0   0   0
## 4: 700.0000         0         0   0   0
##    s.e.response
## 1:            0
## 2:            0
## 3:            0
## 4:            0

wb2spct(Plant_bands())

##     w.length s.e.irrad s.q.irrad Tfr Rfl
##  1: 279.9999         0         0   0   0
##  2: 280.0000         0         0   0   0
## ---
## 21: 739.9999         0         0   0   0
## 22: 740.0000         0         0   0   0
##     s.e.response
##  1:            0
##  2:            0
## ---
## 21:            0
## 22:            0
```

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())

##    w.length s.e.irrad s.q.irrad Tfr Rfl
## 1: 399.9999         0         0   0   0
## 2: 400.0000         0         0   0   0
## 3: 699.9999         0         0   0   0
## 4: 700.0000         0         0   0   0
##    s.e.response wl.color wb.f y
## 1:            0  #03001E   NA 0
## 2:            0  #03001E  PAR 0
## 3:            0  #070000  PAR 0
## 4:            0  #070000   NA 0

wb2tagged_spct(Plant_bands())

##     w.length s.e.irrad s.q.irrad Tfr Rfl
##  1: 279.9999         0         0   0   0
##  2: 280.0000         0         0   0   0
## ---
## 21: 739.9999         0         0   0   0
## 22: 740.0000         0         0   0   0
##     s.e.response wl.color wb.f y
##  1:            0  #000000   NA 0
##  2:            0  #000000  UVB 0
## ---
## 21:            0  #000000   FR 0
## 22:            0  #000000   NA 0
```

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())

##    w.length s.e.irrad s.q.irrad Tfr Rfl
## 1:      550         0         0   0   0
##    s.e.response wl.color wb.f wl.high wl.low y
## 1:            0  #00FF00  PAR     700    400 0

wb2rect_spct(Plant_bands())

##    w.length s.e.irrad s.q.irrad Tfr Rfl
## 1:    297.5         0         0   0   0
## 2:    357.5         0         0   0   0
## 3:    455.0         0         0   0   0
## 4:    535.0         0         0   0   0
## 5:    660.0         0         0   0   0
## 6:    730.0         0         0   0   0
##    s.e.response wl.color  wb.f wl.high wl.low y
## 1:            0  #000000   UVB     315    280 0
## 2:            0  #000000   UVA     400    315 0
## 3:            0  #0000FF  Blue     490    420 0
## 4:            0  #00FF00 Green     570    500 0
## 5:            0  #730000     R     670    650 0
## 6:            0  #010000    FR     740    720 0
```

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.

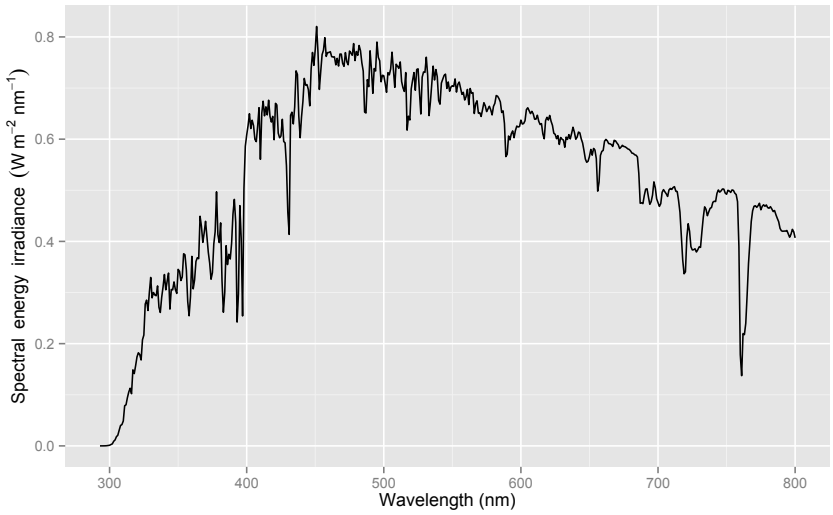
```
attr(wb2rect_spct(PAR()), "spct.tags")

## $time.unit
## [1] "none"
##
## $wb.key.name
## [1] "Bands"
##
## $wl.color
## [1] TRUE
##
## $wb.color
## [1] TRUE
##
## $wb.num
## [1] 1
##
## $wb.colors
## $wb.colors[[1]]
##   PAR.CMF
## "#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 geoms 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.

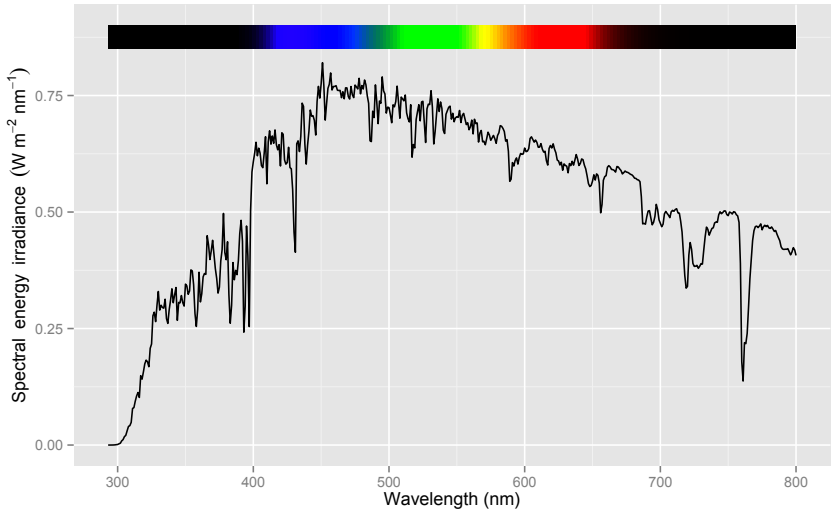
```
fig_sun.z0 <-
  ggplot(data=sun.spct,
```

```
          aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.z0
```



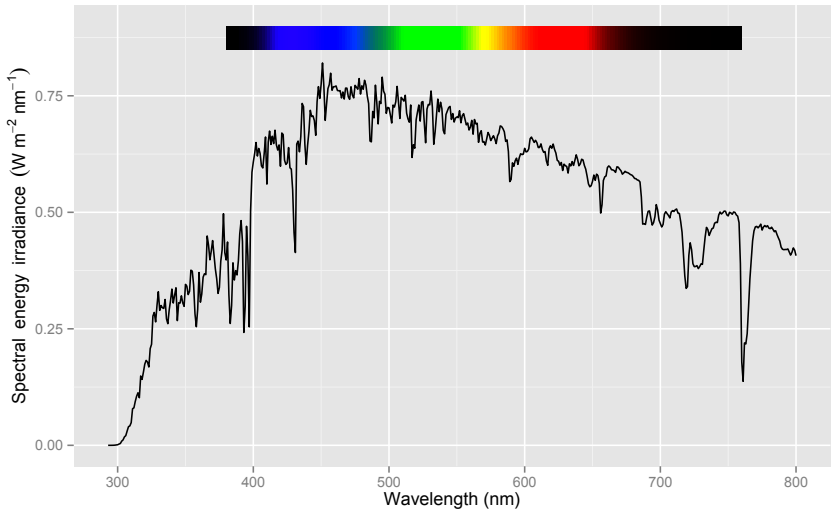
We now add to the plot created above a nearly continuous colour bar for the whole spectrum. To obtain an almost continuous colour scale we use a list of 200 wavebands. We need to specify `color = NA` to prevent the line enclosing each of the 200 rectangles from being plotted. We position the bar at the 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.f),
            color = NA) +
  scale_fill_tgspct(tg.spct=wl.guide.spct)

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.

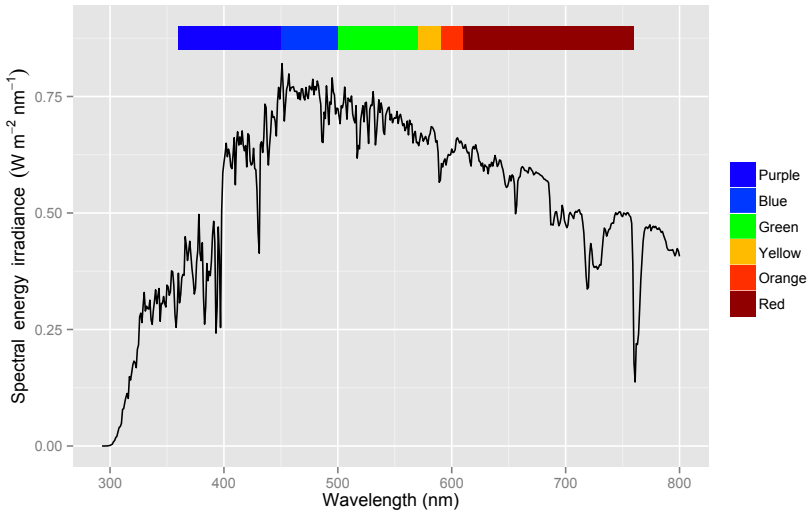
```
wl.guide.spct <- wb2rect_spct(split_bands(VIS(), length.out=200))

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.f),
            color = NA) +
  scale_fill_tgspct(tg.spct=wl.guide.spct)

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.

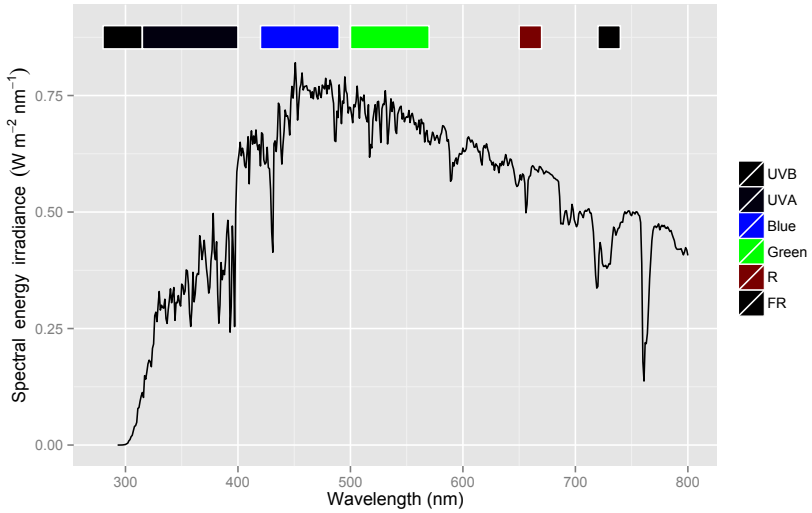
To demonstrate this we replace in the previous example, the previous tagged spectrum with one based on ISO colours. We need to do this replacement in the calls to both `geom_rect` and `scale_fill_tgspct`.

```
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.f),
            color = NA) +
  scale_fill_tgspct(tg.spct=iso.guide.spct)

fig_sun.z3
```



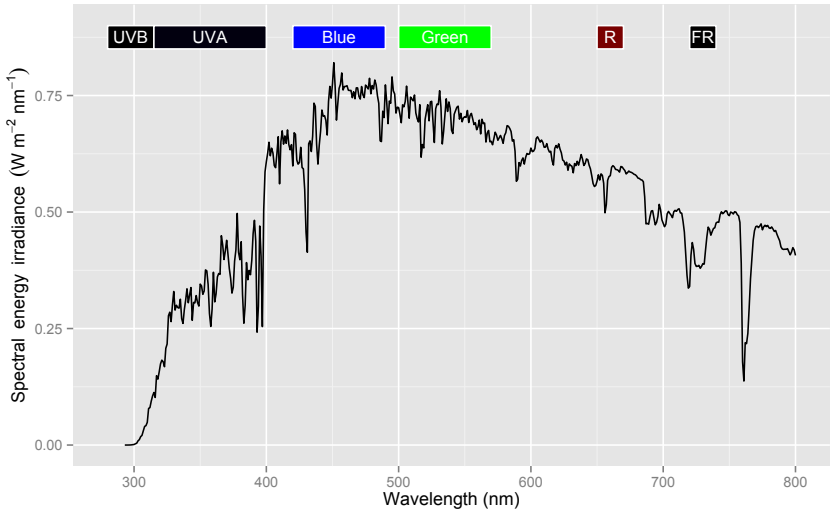
We use as an example plant's sensory colours, to show the case when the wavebands in the list are not contiguous.

```
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.f),
            color = "white") +
  scale_fill_tgspct(tg.spct=plant.guide.spct)

fig_sun.z4
```



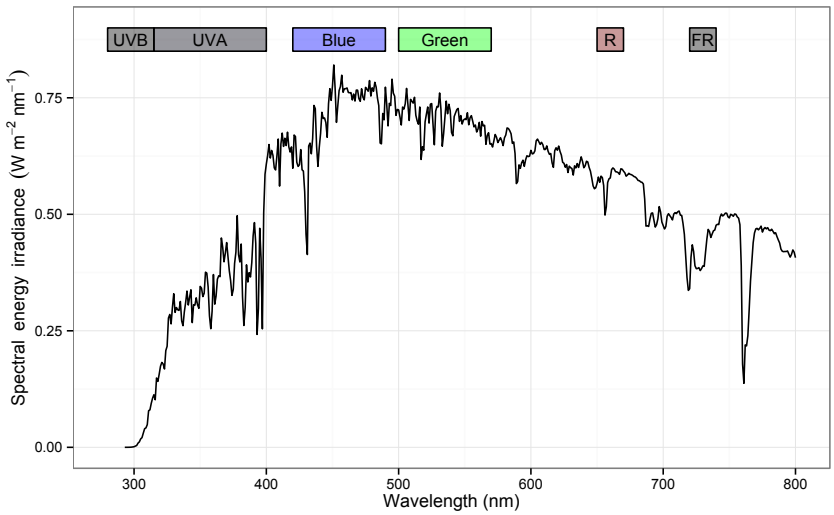
We add text labels on top of the guide, and make the rectangle borders and text white to make the separation between the different 'invisible' wavebands clear. As we are adding labels, the 'guide' or key becomes redundant and we remove it by adding `guide="none"` to the fill scale.

```
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.f),
            color = "white") +
  geom_text(data=plant.guide.spct,
            aes(y = y + 0.875, label = as.character(wb.f)),
            color = "white", size=4) +
  scale_fill_tgspct(tg.spct=plant.guide.spct, guide="none")

fig_sun.z5
```



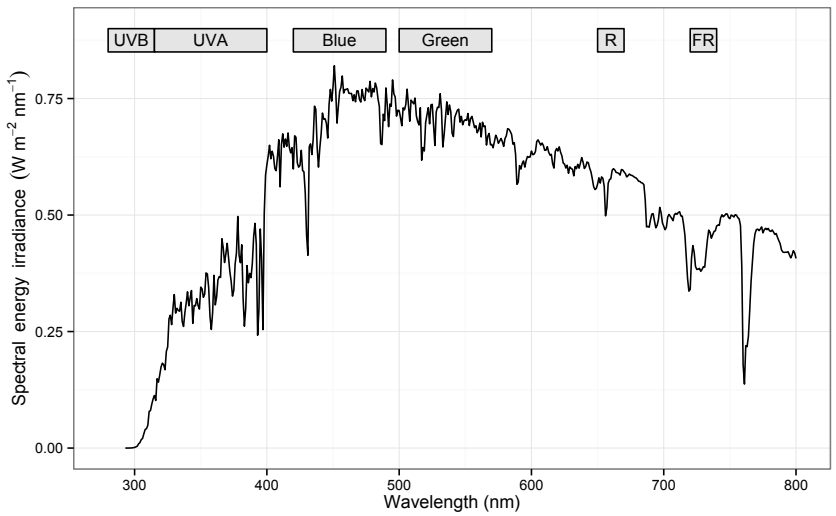
Here we add `alpha` or transparency to make the colours paler, and use black text and lines.

```
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.f),
        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_tgspct(tg.spct=plant.guide.spct, guide="none")

fig_sun.z6 + theme_bw()
```



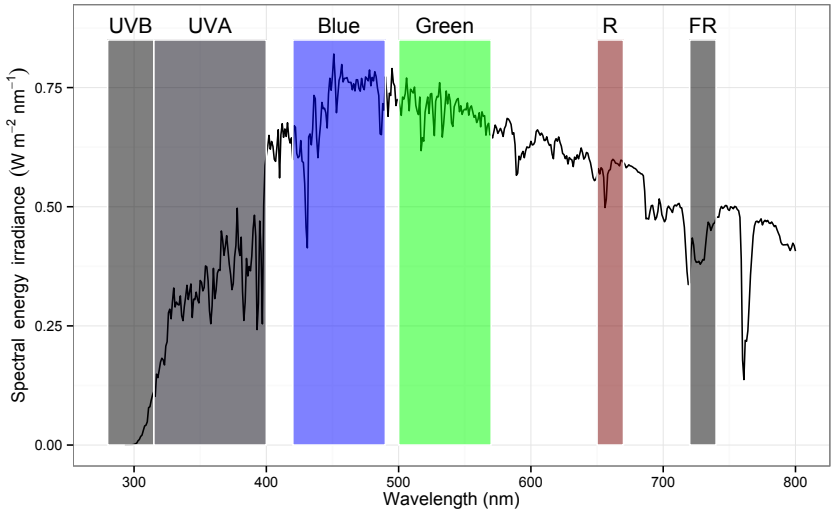
We change the guide so that all rectangles are filled with the same shade of grey by moving `fill` out of `aes` and setting it to a constant.

```
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()
```



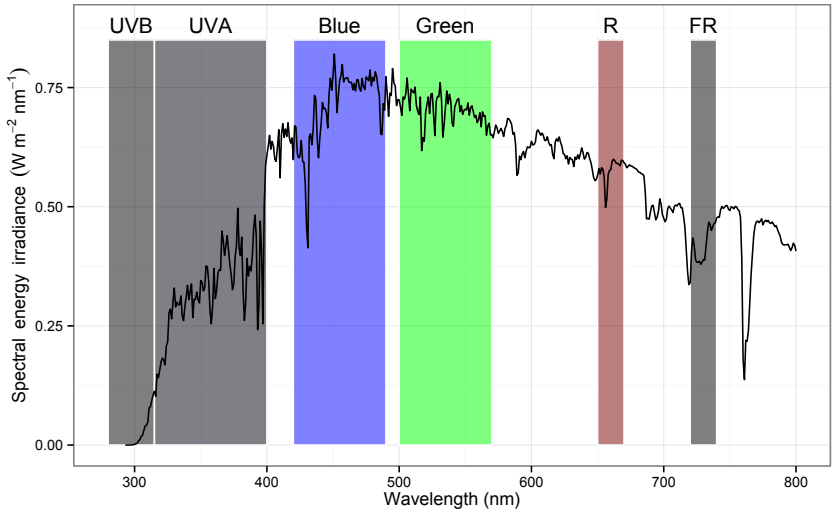
We can obtain annotations similar to those in ?? in page ?? created with `annotate_waveband` using geoms.

```
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.f),
        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_tgspct(tg.spct=plant.guide.spct, guide="none")

fig_sun.z8 + theme_bw()
```



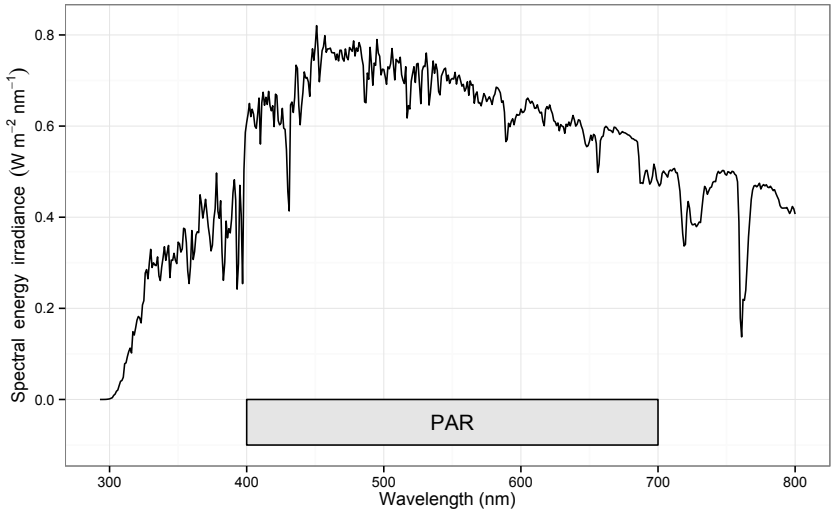
The example above can be improved by changing the order in which the geoms are added. In the plot above we can see that the rectangles are plotted on top of the line for the spectral irradiance. By changing the order we obtain a better plot.

```
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.f),
       color = "white", alpha=0.5) +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f)),
       color = "black") +
  geom_line() +
  scale_fill_tgspct(tg.spct=plant.guide.spct, guide="none") +
  labs(
    y = ylab_watt,
    x = "Wavelength (nm)")

fig_sun.z8a + theme_bw()
```



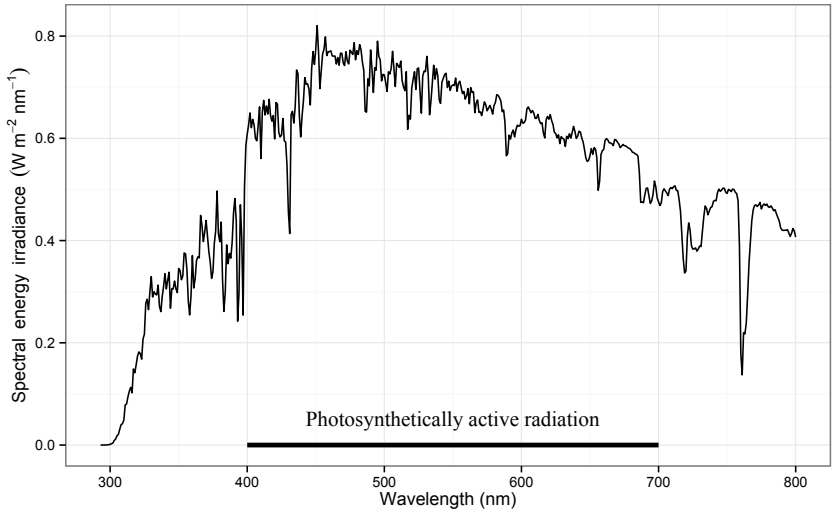
In the examples above we used predefined lists of wavebands, but one can, of course, use any list of waveband definitions, for example explicitly created with `list` and `new_waveband`, or `list` and any combination of user-defined and predefined wavebands. Even single waveband definitions are allowed.

```
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()
```



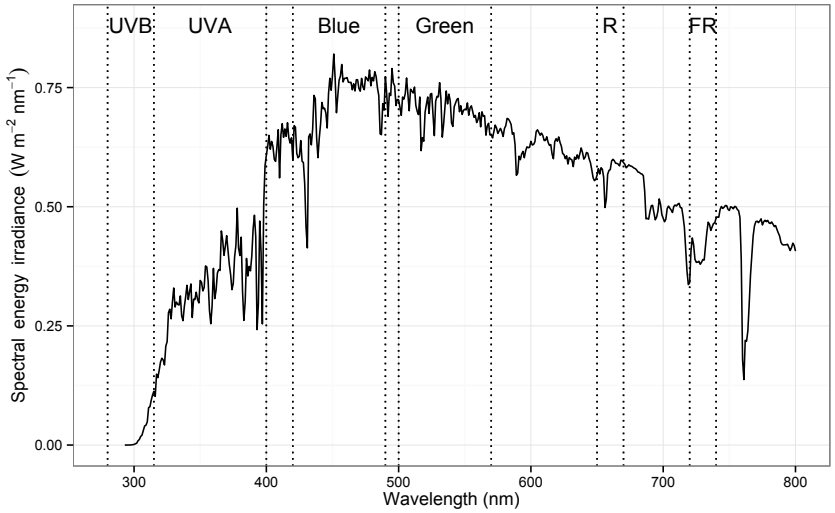
We can also use `geom_segment` to draw lines, including arrows. In this example we also set a different font `family` and label text. We can replace the label text which is by default obtained from the waveband definition by assigning a name to the waveband as member of the list. We use single quotes 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()
```



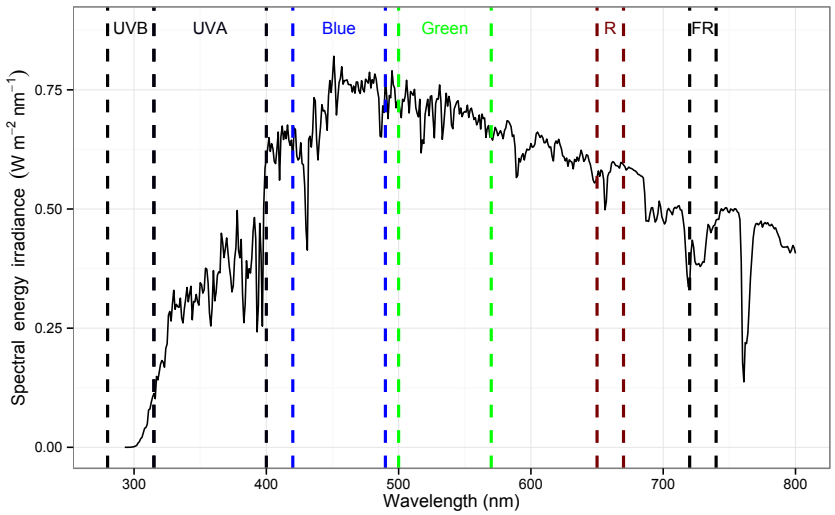
In this section we have used until now function `wb2rect_spct` to create 'spectral' annotation data from waveband definitions. Two other functions are available, that are needed or easier to use in some cases. One such case is when we have a list of wavebands and we would like to mark their boundaries 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()
```



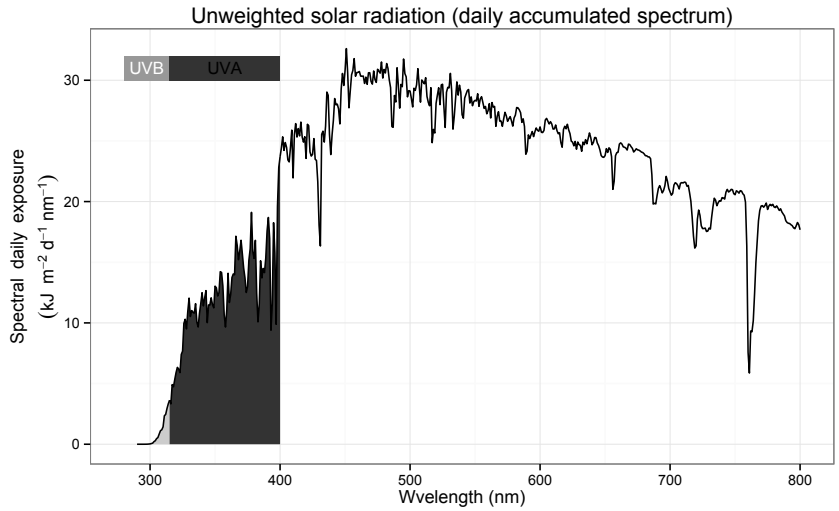
Function `wb2tagged_spct` returns the same data as `wb2spct` but 'tagged'. As shown in the next code chunk, tagging allows us to use waveband-dependent colours to the vertical lines.

```
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.f),
             size=1, linetype="dashed") +
  geom_text(data=plant.guide.spct,
       aes(y = y + 0.88, label = as.character(wb.f), colour=wb.f),
       size=4) +
  scale_colour_tgspct(tg.spct=plant.guide.spct, guide="none")

fig_sun.z12 + theme_bw()
```



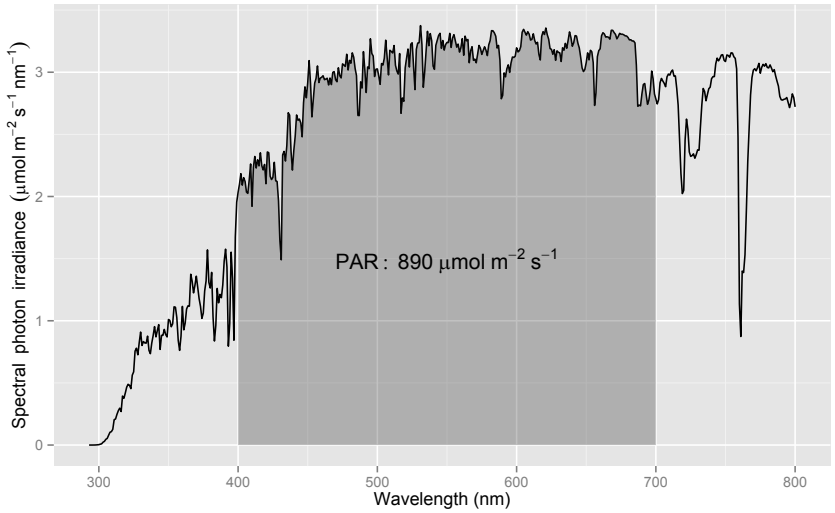
Of course it is possible to combine tagged data spectra and tagged spectra created from wavebands. The tagging is consistent, so, as demonstrated in the next figure, the same aesthetic 'link' works for both spectra. In this case the fill scale and the setting of fill to `wb.f` work accross different '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 earleir 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 <- sun.daily.spct
tag(my.sun.spct, list(UVB(), UVA()))

##      w.length    s.e.irrad    s.q.irrad wl.color
##   1:      290 0.000000e+00 0.000000e+00  #000000
##   2:      291 1.788149e-04 4.349734e-10  #000000
##  ---
## 512:      799 1.808827e+04 1.208119e-01  #000000
## 513:      800 1.767467e+04 1.181973e-01  #000000
##           wb.f
##   1: UVB.tr.lo
##   2: UVB.tr.lo
##  ---
## 512:        NA
## 513:        NA

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 = "Wvelength (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("white","black"), size=4) +
  theme_bw()

fig_sun.uv1
```

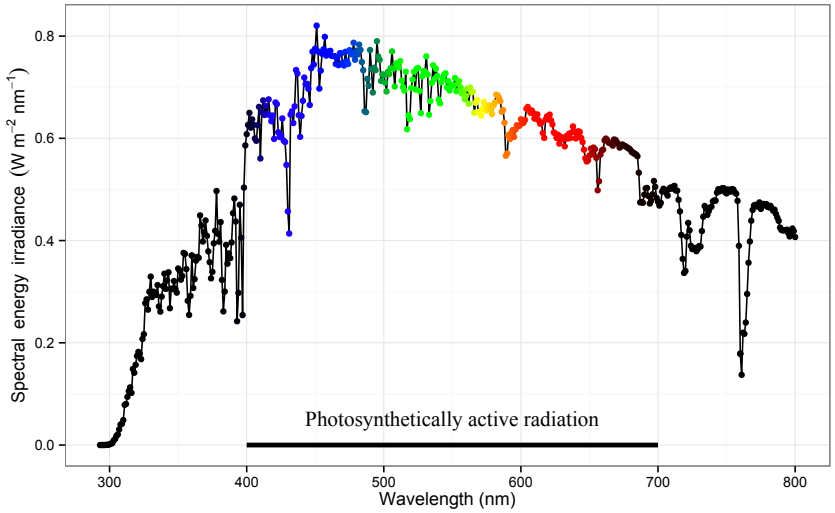


Possible variations are almost endless, so we invite the reader to continue exploring how the functions from package `photobiology` can be used together with `ggplot`, to obtain beautiful plots of spectra. As an example here we show new versions of two plots from the previous section, one using a filled 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)") +
  annotate_waveband(PAR(), "text",
                    label=paste("PAR:~", signif(par,digits=2),
                                " * ~mu * mol~m^{-2}~s^{-1}", sep=""),
                    y=1.5, colour="black", size=5, parse=TRUE)

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()
```

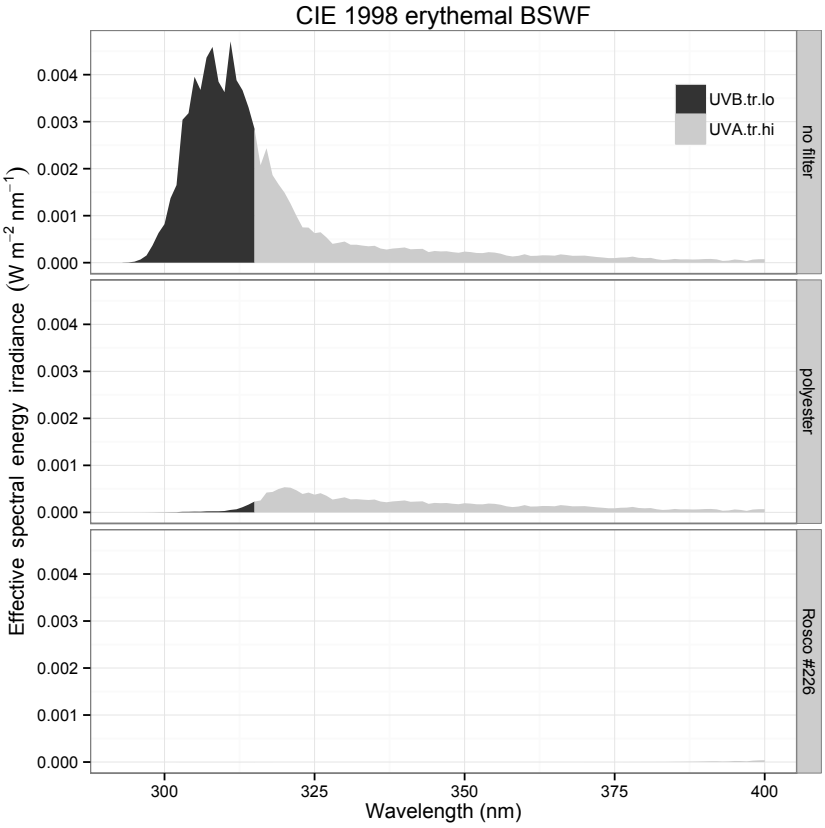


15.11 Task: plotting effective spectral irradiance

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 <- sun.spct * CIE()
sun.eff.cie.pe.spct <- sun.spct * polyester.new.spct * CIE()
sun.eff.cie.226.spct <- sun.spct * uv.226.new.spct * CIE()
tag(sun.eff.cie.nf.spct, UV_bands())

##      w.length    s.e.irrad wl.color      wb.f
##   1: 293.0000 2.609665e-06  #000000 UVB.tr.lo
##   2: 294.0000 6.142401e-06  #000000 UVB.tr.lo
##  ---
## 109: 399.9989 7.395673e-05  #03001E UVA.tr.hi
## 110: 399.9990 7.395674e-05  #03001E        NA

tag(sun.eff.cie.pe.spct, UV_bands())

##      w.length    s.e.irrad wl.color      wb.f
##   1: 293.0000 7.828995e-09  #000000 UVB.tr.lo
##   2: 294.0000 1.842720e-08  #000000 UVB.tr.lo
##  ---
## 109: 399.9989 6.752241e-05  #03001E UVA.tr.hi
## 110: 399.9990 6.752244e-05  #03001E        NA

tag(sun.eff.cie.226.spct, UV_bands())

##      w.length    s.e.irrad wl.color      wb.f
##   1: 293.0000 2.609665e-11  #000000 UVB.tr.lo
##   2: 294.0000 6.142401e-11  #000000 UVB.tr.lo
##  ---
## 109: 399.9989 3.863952e-05  #03001E UVA.tr.hi
## 110: 399.9990 3.863980e-05  #03001E        NA
```

```
invisible(sun.eff.cie.nf.spct[ , filter := 'no filter'])
invisible(sun.eff.cie.pe.spct[ , filter := 'polyester'])
invisible(sun.eff.cie.226.spct[ , filter := 'Rosco #226'])
sun.eff.cie.spct <- rbindspct(list(sun.eff.cie.nf.spct,
                                   sun.eff.cie.pe.spct,
                                   sun.eff.cie.226.spct))
invisible(sun.eff.cie.spct[ , filter := factor(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 eficiency

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.

15.12 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.new.spct * CIE(),
                        list(UVB(), UVA()))
cie.226.irrad <- e_irrad(sun.spct * uv.226.new.spct * CIE(),
                         list(UVB(), UVA()))
```

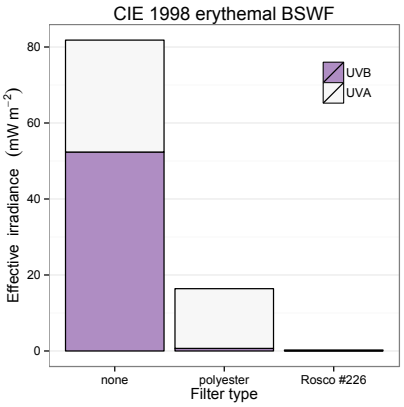
We assemble a data table by concatenating the irradiance and adding factors for filter type and wave bands. When defining the factors, we use `levels` to make sure that the levels are ordered as we would like to plot them.

```
cie.dt <- data.table(
  cie.irrad = c(cie.nf.irrad, cie.pe.irrad, cie.226.irrad),
  filter = factor(rep(c('none', 'polyester', 'Rosco #226'), c(2,2,2)),
                  levels=c('none', 'polyester', 'Rosco #226')),
  w.band = factor(rep(c('UVB', 'UVA'), 3),
                  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.

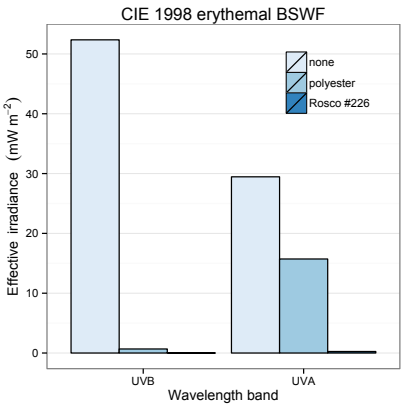
```
cie.dt

##       cie.irrad     filter w.band
## 1: 5.235708e-02       none    UVB
## 2: 2.945736e-02       none    UVA
## 3: 6.758170e-04  polyester    UVB
## 4: 1.572018e-02  polyester    UVA
## 5: 5.235708e-07 Rosco #226    UVB
## 6: 2.539816e-04 Rosco #226    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
```



15.13 Task: plotting a spectrum using colour bars

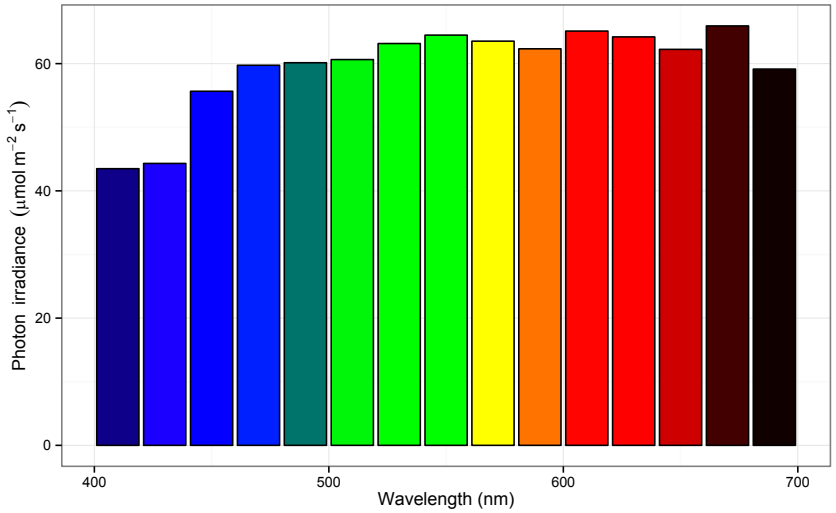
We show now the last example, related to the ones above, but creating a bar plot with more bars. First we calculate photon irradiance for different equally spaced bands within PAR using function `split_bands`. The code is written so that by changing the first two lines you can adjust the output.

```
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.table(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.

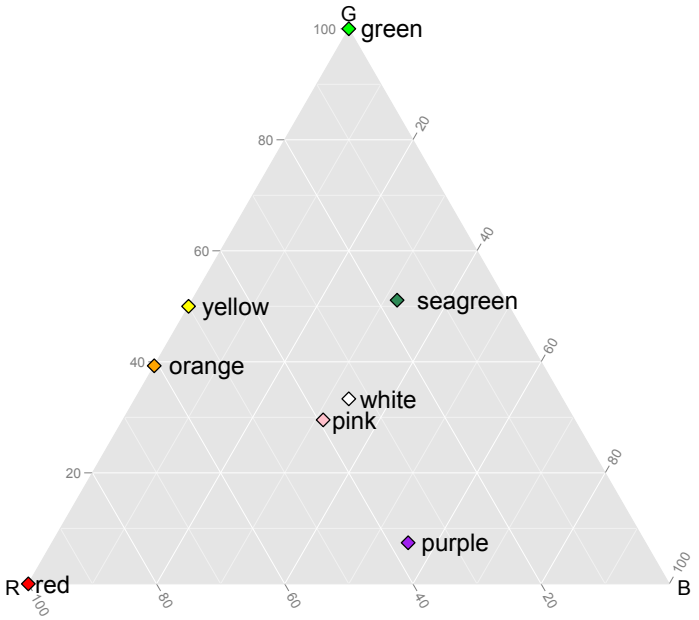
15.14 Task: plotting colours in Maxwell's triangle

15.14.1 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`. Geoms, 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
```



15.15 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 example, 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:photobiologygg))
try(detach(package:ggtern))
try(detach(package:ggplot2))
try(detach(package:gridExtra))
try(detach(package:photobiologyFilters))
try(detach(package:photobiologyWavebands))
try(detach(package:photobiology))
```

CHAPTER 16

Radiation physics

Abstract

In this chapter we explain how to code some optics and physics computations in R.

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(photobiologygg)

## Loading required package:  photobiologyWavebands
##
## Attaching package:  'photobiologygg'
##
## The following objects are masked _by_ '.GlobalEnv':
##
##    scale_colour_tgspct, scale_fill_tgspct

library(photobiology)
library(photobiologyFilters)
```

16.2 Introduction

16.3 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):

$$L_s(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{e^{(hc/k_B T\lambda)} - 1} \tag{16.1}$$

with Boltzmann's constant $k_B = 1.381 \times 10^{-23}$ JK^{-1}, Planck's constant $h = 6.626 \times 10^{-34}$ Js and speed of light in vacuum $c = 2.998 \times 10^{8}$ ms^{-1}.

We can easily define an R function based on the equation above, which returns $W sr^{-1} m^{-3}$:

```
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 vectorized:

```
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]:

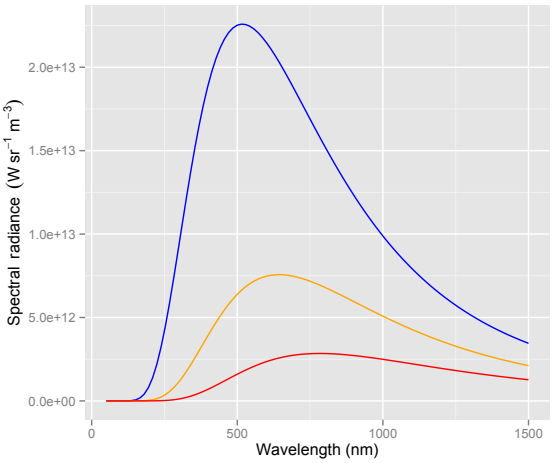
```
black_body_spectrum(c(500, 500, 600, 600), c(4500,5000)) # tricky!

## [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),
```

[1] Exercise: calculate each of the four values individually to work out how the two vectors are being used.

```
                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)")
```



Wien's displacement law, gives the peak wavelength of the radiation emitted by a black body as a function of its absolute temperature.

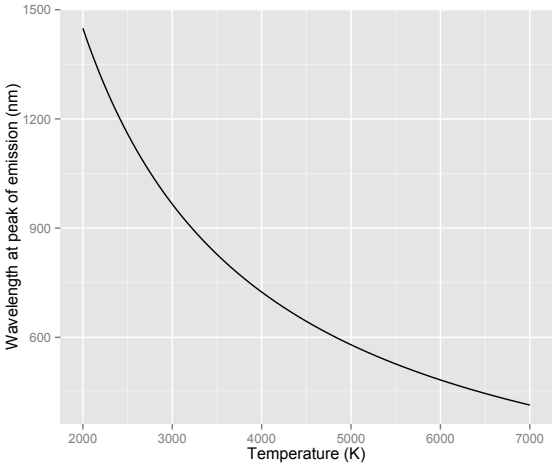
$$\lambda_{max} \cdot T = 2.898 \times 10^6 \,\mathrm{nm\,K} \tag{16.2}$$

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:photobiologygg))
try(detach(package:photobiology))
try(detach(package:ggplot2))
```

Part III

Catalogue of data sources

Part IV

Data acquisition and modelling

CHAPTER 17

Further reading about R

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Build information

```
Sys.info()
```

```
##                      sysname
##                    "Windows"
##                      release
##                      "7 x64"
##                      version
## "build 7601, Service Pack 1"
##                     nodename
##                      "MUSTI"
##                      machine
##                     "x86-64"
##                        login
##                     "aphalo"
##                         user
##                     "aphalo"
##               effective_user
##                     "aphalo"
```

```
sessionInfo()
```

```
## R version 3.2.0 (2015-04-16)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 7 x64 (build 7601) Service Pack 1
##
## locale:
## [1] LC_COLLATE=English_United Kingdom.1252
## [2] LC_CTYPE=English_United Kingdom.1252
## [3] LC_MONETARY=English_United Kingdom.1252
## [4] LC_NUMERIC=C
## [5] LC_TIME=English_United Kingdom.1252
##
## attached base packages:
## [1] grid      methods   tools     stats
```

```
## [5] graphics  grDevices utils     datasets
## [9] base
##
## other attached packages:
## [1] photobiologyWavebands_0.3.1.9000
## [2] photobiologySun_0.3.2
## [3] scales_0.2.5
## [4] proto_0.3-10
## [5] photobiology_0.6.8
## [6] data.table_1.9.4
## [7] stringr_1.0.0
## [8] knitr_1.10.5
##
## loaded via a namespace (and not attached):
##  [1] Rcpp_0.11.6
##  [2] RColorBrewer_1.1-2
##  [3] formatR_1.2
##  [4] plyr_1.8.3
##  [5] highr_0.5
##  [6] bitops_1.0-6
##  [7] photobiologyFilters_0.3.0.9000
##  [8] photobiologyLEDs_0.3.0
##  [9] photobiologyLamps_0.3.0.90000
## [10] digest_0.6.8
## [11] lattice_0.20-31
## [12] lubridate_1.3.3
## [13] evaluate_0.7
## [14] memoise_0.2.1
## [15] gtable_0.1.2
## [16] photobiologygg_0.3.3
## [17] png_0.1-7
## [18] mapproj_1.2-2
## [19] ggtern_1.0.5.0
## [20] gridExtra_0.9.1
## [21] maps_2.3-9
## [22] RgoogleMaps_1.2.0.7
## [23] caTools_1.17.1
## [24] jpeg_0.1-8
## [25] RJSONIO_1.3-0
## [26] sp_1.1-1
## [27] ggmap_2.4
## [28] ggplot2_1.0.1
## [29] reshape2_1.4.1
## [30] splus2R_1.2-0
## [31] magrittr_1.5
## [32] photobiologyReflectors_0.3.0
## [33] MASS_7.3-40
## [34] colorspace_1.2-6
## [35] geosphere_1.3-13
## [36] labeling_0.3
## [37] stringi_0.4-1
## [38] munsell_0.4.2
## [39] rjson_0.2.15
## [40] chron_2.3-45
```