

# R for Photobiology

*A handbook*

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## Preface

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

### Acknowledgements

We thank Titta Kotilainen, Stefano Catola, and ... for very useful comments and suggestions.



## List of abbreviations and symbols

For quantities and units used in photobiology we follow, as much as possible, the recommendations of the Commission Internationale de l'Éclairage as described by Sliney2007.

Symbol	Definition
$\alpha$	(%).
$\Delta e$	water vapour pressure difference (Pa).
$\epsilon$	emittance ( $\text{W m}^{-2}$ ).
$\lambda$	wavelength (nm).
$\theta$	solar zenith angle (degrees).
$\nu$	frequency (Hz or $\text{s}^{-1}$ ).
$\rho$	(%).
$\sigma$	Stefan-Boltzmann constant.
$\tau$	(%).
$\chi$	water vapour content in the air ( $\text{g m}^{-3}$ ).
$A$	(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 ( $\text{W m}^{-2}$ ).
$E(\lambda)$	spectral (energy) irradiance ( $\text{W m}^{-2} \text{ nm}^{-1}$ ).

$E_0$	fluence rate, also called scalar irradiance ( $\text{W m}^{-2}$ ).
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 abbreviated as GPAS Caldwell1971.
GEN(G)	mathematical formulation of GEN by Green1974 .
GEN(T)	mathematical formulation of GEN by Thimijan1978.
$h$	Planck's constant.
$h'$	Planck's constant per mole of photons.
$H$	exposure, frequently called dose by biologists ( $\text{kJ m}^{-2} \text{d}^{-1}$ ).
$H^{\text{BE}}$	biologically effective (energy) exposure ( $\text{kJ m}^{-2} \text{d}^{-1}$ ).
$H_p^{\text{BE}}$	biologically effective photon exposure ( $\text{mol m}^{-2} \text{d}^{-1}$ ).
HPS	high pressure sodium, a type of discharge lamp.
HSD	honestly significant difference.
$k_B$	Boltzmann constant.
$L$	radiance ( $\text{W sr}^{-1} \text{m}^{-2}$ ).
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 ( $Q_{\text{PAR}}$ ).
PTFE	polytetrafluoroethylene.
PVC	polyvinylchloride.
$q$	energy in one photon ('energy of light').
$q'$	energy in one mole of photons.
$Q$	photon irradiance ( $\text{mol m}^{-2} \text{s}^{-1}$ or $\mu\text{mol m}^{-2} \text{s}^{-1}$ ).
$Q(\lambda)$	spectral photon irradiance ( $\text{mol m}^{-2} \text{s}^{-1} \text{nm}^{-1}$ or $\mu\text{mol m}^{-2} \text{s}^{-1} \text{nm}^{-1}$ ).
$r_0$	distance from sun to earth.
RAF	(nondimensional).
RH	relative humidity (%).
$s$	energy effectiveness (relative units).

$s(\lambda)$	spectral energy effectiveness (relative units).
$s^p$	quantum effectiveness (relative units).
$s^p(\lambda)$	spectral quantum effectiveness (relative units).
s.d.	standard deviation.
SDK	software development kit.
s.e.	standard error of the mean.
SR	spectroradiometer.
$t$	time.
$T$	temperature.
TUV	tropospheric UV.
$U$	electric potential difference or voltage (e.g. sensor output in V).
UV	ultraviolet radiation ( $\lambda = 100\text{--}400\text{ nm}$ ).
UV-A	ultraviolet-A radiation ( $\lambda = 315\text{--}400\text{ nm}$ ).
UV-B	ultraviolet-B radiation ( $\lambda = 280\text{--}315\text{ nm}$ ).
UV-C	ultraviolet-C radiation ( $\lambda = 100\text{--}280\text{ nm}$ ).
$UV^{BE}$	biologically effective UV radiation.
UTC	coordinated universal time, replaces GMT in technical use.
VIS	radiation visible to the human eye ( $\approx 400\text{--}700\text{ nm}$ ).
WMO	World Meteorological Organization.
VPD	water vapour pressure deficit (Pa).
WOUDC	World Ozone and Ultraviolet Radiation Data Centre.



## **Part I**

### **Getting ready**



C H A P T E R



## Introduction

### Abstract

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

### 1.1 Radiation and molecules



CHAPTER



## Optics

### **Abstract**

In this chapter we explain how to .

### **2.1 Task:**



CHAPTER



## Photochemistry

### Abstract

In this chapter we explain how to .

### 3.1 Task:



CHAPTER



## 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.

### 4.1 Task:

### 4.2 Introduction

All the software used for typesetting this handbook and developing the *r4photobiology* software suite is free and open source. All the software used 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 on a Linux server, 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 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 step is to use a text editor which integrates to some extent with R, but still this is not ideal. 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 important in the case of errors and ‘debugging’. We also use a *LAT<sub>E</sub>X* for typesetting. Is what we used for the handbook, and what we routinely for reporting data analyses, and that PJA also uses for all ‘overhead’ slides he writes. You, do not need to go this far to be able to profit from R and our suite, but the set up we will describe here, is what we currently use, in this by far the best one we have used 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 many alternatives and the only piece that you cannot replace is R itself.

### 4.3 The different pieces

#### 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 in a programming language, and being able to call and being called by programs and subroutine libraries, makes it 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 released versions of packages are kept. Packages can be installed and updated from CRAN and similar repositories directly from within R.

In you are not familiar with R, please, go through the Appendixes A, B and C, before delving into our 'Cook Book'.

#### 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.

#### Version control: Git and Subversion

Version control systems help with keeping track of the history of software development, data analysis, or even manuscript writing. They make it possible for several programmers, analysts, authors and or editors to work on the same files in parallel and then merge their edits. They also allow easy transfer of the whole 'projects' between computers. Git is very popular, and Github and Bitbucket are popular hosts for repositories.

#### 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.

**L<sup>A</sup>T<sub>E</sub>X**

L<sup>A</sup>T<sub>E</sub>X is built on top of T<sub>E</sub>X. T<sub>E</sub>X code and features were ‘frozen’ (only bugs are fixed) long ago. There are currently a few ‘improved’ derivatives: pdfT<sub>E</sub>X, X<sub>E</sub>T<sub>E</sub>X, and LuaT<sub>E</sub>X. Currently the most popular T<sub>E</sub>X in western countries is pdftex which can directly output PDF files. X<sub>E</sub>T<sub>E</sub>X can handle text both written from left to right and right to left, even in the same document, and is the most popular T<sub>E</sub>X engine in China and other Asian countries.



## 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 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).

One of the main difficulties when working with spectral data is that one may need to operate on data sets measured at different wavelength values and steps sizes. The functions in the suite handle any mismatch by interpolation before applying operations or functions. Although by default 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`, and photon spectral irradiance `s.q.irrad`<sup>1</sup>.

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  $\text{W m}^{-2} \text{nm}^{-1}$  yields an output in  $\text{mol m}^{-2} \text{s}^{-1} \text{nm}^{-1}$  rather than  $\mu\text{mol m}^{-2} \text{s}^{-1} \text{nm}^{-1}$ ).

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.

---

<sup>1</sup>q derives from ‘quantum’.

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
• photobiology	functions	basic functions and example data
• photobiologyVIS	definitions	quantification of VIS radiation
• photobiologyUV	definitions	quantification of UV radiation
• 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 broadband sensors
• photobiologyPhy	functs + data	phytochromes
• photobiologyCry	functs + data	cryptochromes
• photobiologyPhot	functs + data	phototropins
• photobiologyUVR8	functs + data	phototropins
• photobiologygg	funtions	extensions to package <code>ggplot2</code>
• rTUV	functs + data	TUV model interface
• rOmniDriver	functions	control of Ocean Optics spectrometers

## 5.2 `r4photo` repository

I have created a small repository for the packages. This repository follows the CRAN folder structure, so now package installation can be done using just the 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 `r4photo` 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 `r4photo` 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(photoCRAN =
                           "http://www.mv.helsinki.fi/aphalo/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(photoCRAN =
                           "http://www.mv.helsinki.fi/aphalo/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’. 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. The minimum needed is.

```
utils::setRepositories(graphics =getOption("menu.graphics"),
                      ind = c(1, 6),
                      addURLs = c(photoCRAN =
                        "http://www.mv.helsinki.fi/aphalo/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. 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 r4photo repository as shown above, the photobiology packages can be installed and uninstalled through the normal RStudio menus and dialogues. 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 with:

```
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.

### 5.3 How to install the packages

The examples given in this page assume that r4photo is not in the list of repositories known to the current R session. See the section 5.2 on the r4photo repository for an alternative to the approach given here.

To install the latest version of one package (photobiology used as example) you just need to indicate the repository. However this simple command will only install the dependencies between the different photobiology packages.

```
install.packages("photobiology",
                 repos = "http://www.mv.helsinki.fi/aphalo/R")
```

To update what is already installed, this command is enough (even if the packages have been installed manually before):

```
update.packages(repos = "http://www.mv.helsinki.fi/aphalo/R")
```

The best way to install the packages is to specify both my repository and a normal CRAN repository, then all dependencies will be automatically installed. The new package photobiologyAll just loads and imports all the packages in the suite, except for photobiologygg. Because of this dependency all the packages are installed unless already installed.

```
install.packages(c("photobiologyAll", "photobiologygg"),
  repos = c(photoCRAN =
    "http://www.mv.helsinki.fi/aphalo/R",
    CRAN =
    "http://cran.rstudio.com"))
```

```
install.packages(c("photobiologyAll", "photobiologygg"),
  repos = c(photoCRAN =
    "http://www.mv.helsinki.fi/aphalo/R",
    CRAN =
    "http://cran.rstudio.com"))
```

This example also shows how one can use an array of package names (in this example all my currently available photobiology packages) in the call to the function `install.packages`, this is useful if you want to install only a subset of the files, or if you want to make sure that any older install of the packages is overwritten:

```
photobiology_packages <- c("photobiology",
  "photobiologyVIS", "photobiologyUV",
  "photobiologyCry", "photobiologyPhy",
  "photobiologyLamps", "photobiologyLEDs",
  "photobiologySun", "photobiologygg",
  "photobiologyFilters", "photobiologySensors")

install.packages(photobiology_packages,
  repos = c(photoCRAN =
    "http://www.mv.helsinki.fi/aphalo/R",
    CRAN =
    "http://cran.rstudio.com"))
```

The commands above install all my packages and all their dependencies from CRAN if needed. The following command will update all the packages currently installed (if new versions are available) and install any new dependencies.

```
update.packages(repos =
  c(photoCRAN =
    "http://www.mv.helsinki.fi/aphalo/R",
    CRAN =
    "http://cran.rstudio.com"))
```

The instructions above should work under Windows as long as you have a supported version of R (3.0.0 or later) because I have built suitable binaries, under other OS you may need to add `type="source"` unless this is already the

default. We will try to build OS X binaries for Mac so that installation is easier. Meanwhile if installation fails try adding type="source" to the commands given above. For example the first one would become:

```
install.packages("photobiology",
  repos = "http://www.mv.helsinki.fi/aphalo/R",
  type="source")
```

When using type=source you may need to install some dependencies like the splus2R package beforehand from CRAN if building it from sources fails.



**Part II**

**Cookbook**





CHAPTER  
6

## Radiation physics

### Abstract

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

### 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(ggplot2)
library(photobiologygg)
library(photobiology)
library(photobiologyFilters)
```

### 6.2 Introduction

### 6.3 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):

$$L_s(\lambda, T) = \frac{2hc^2}{\lambda^5} \cdot \frac{1}{e^{(hc/k_B T \lambda)} - 1} \quad (6.1)$$

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  $c = 2.998 \times 10^8$  m s $^{-1}$ .

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] 1.212e+13

```

The function is vectorized:

```

black_body_spectrum(c(300,400,500), 5000)
## [1] 3.355e+12 8.759e+12 1.212e+13

```

```

black_body_spectrum(500, c(4500,5000))
## [1] 6.388e+12 1.212e+13

```

We aware that if two vectors are supplied, then the elements in each one are matched and recycled<sup>1</sup>:

```

black_body_spectrum(c(500, 500, 600, 600), c(4500,5000)) # tricky!
## [1] 6.388e+12 1.212e+13 7.475e+12 1.278e+13

```

We can use the function defined above for plotting black body emission spectra for different temperatures. We use `ggplot2` and directly plot a function using `stat_function`, using `args` to pass the additional argument giving the absolute temperature to be used. We plot three lines using three different temperatures (5600 K, 4500 K, and 3700 K):

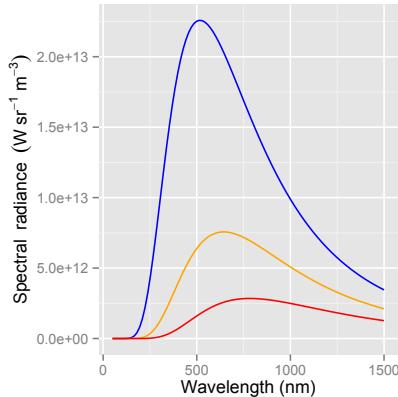
```

ggplot(data=data.frame(x=c(50,1500)), aes(x)) +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=5600),
                colour="blue") +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=4500),
                colour="orange") +
  stat_function(fun=black_body_spectrum,
                args = list(Tabs=3700),
                colour="red") +
  labs(y=expression(Spectral~radianc~(W~sr^-1~m^-3)),
       x="Wavelength (nm)")

```

---

<sup>1</sup>Exercise: calculate each of the four values individually to work out how the two vectors are being used.



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

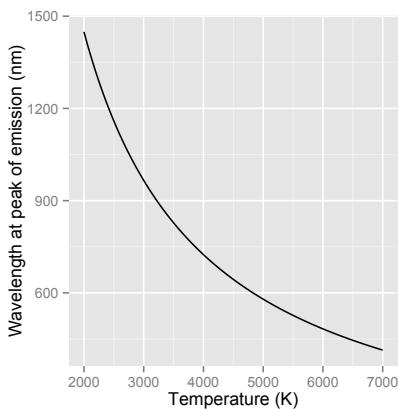
$$\lambda_{max} \cdot T = 2.898 \times 10^6 \text{ nm K} \quad (6.2)$$

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)")
```





## Astronomy

### Abstract

In this chapter we explain how to code some astronomical computations 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(lubridate)
library(ggplot2)
library(ggmap)
```

### 7.2 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 calcualtions 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("20032014")
## [1] "2014-03-20 UTC"

mdy("03202014")
## [1] "2014-03-20 UTC"
```

For astronomical calculations we 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 inputting coordinate values manually, they should in degrees as numeric values (in other words the fractional part is given as part of floating point number in degrees, and not as separate integers representing minutes and seconds of degree).

```
geocode("Helsinki")
##      lon    lat
## 1 24.94 60.17

geocode("Viikinkaari 1, 00790 Helsinki, Finland")
##      lon    lat
## 1 25.02 60.23
```

### 7.3 Task: calculating the length of the photoperiod

In function `day_night` from our `photobiology` package we use function `sun_angles`, which is an edited version of function `sunAngle` from package `ode`, to calculate the altitude or 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_night` returns a list containing the times at sunrise, sunset and noon, and day- and night lengths. 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")
geo_code_BA

##      lon    lat
## 1 -58.38 -34.6

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 UTC"
##
## $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
## Time difference of 14.33 hours
##
## $nightlength
## Time difference of 9.675 hours

day_night(ymd("2013-06-21"),
          lon = geo_code_BA[["lon"]],
          lat = geo_code_BA[["lat"]],
          tz="America/Argentina/Buenos_Aires")

## $day
## [1] "2013-06-21 UTC"
##
## $sunrise
## [1] "2013-06-21 08:04:57 ART"
##
## $noon
## [1] "2013-06-21 12:55:32 ART"
##
## $sunset
## [1] "2013-06-21 17:45:49 ART"
##
## $daylength
## Time difference of 9.681 hours
```

```
##  
## $nightlength  
## Time difference of 14.32 hours
```

We here repeat the same calculations for Munich on the same days —note that the output for December is in "EET" time coordinates, and for June it is in "EEST", i.e. in ‘winter-’ and ‘summer time’ coordinates.

```
geo_code_Mu <- geocode("Munich")  
geo_code_Mu  
  
##      lon   lat  
## 1 11.58 48.14  
  
day_night(ymd("2013-12-21"),  
          lon = geo_code_Mu[["lon"]],  
          lat = geo_code_Mu[["lat"]],  
          tz="Europe/Berlin")  
  
## $day  
## [1] "2013-12-21 UTC"  
##  
## $sunrise  
## [1] "2013-12-21 08:07:27 CET"  
##  
## $noon  
## [1] "2013-12-21 12:11:49 CET"  
##  
## $sunset  
## [1] "2013-12-21 16:16:11 CET"  
##  
## $daylength  
## Time difference of 8.146 hours  
##  
## $nightlength  
## Time difference of 15.85 hours  
  
day_night(ymd("2013-06-21"),  
          lon = geo_code_Mu[["lon"]],  
          lat = geo_code_Mu[["lat"]],  
          tz="Europe/Berlin")  
  
## $day  
## [1] "2013-06-21 UTC"  
##  
## $sunrise  
## [1] "2013-06-21 05:19:41 CEST"  
##  
## $noon  
## [1] "2013-06-21 13:15:29 CEST"  
##  
## $sunset  
## [1] "2013-06-21 21:11:16 CEST"  
##  
## $daylength  
## Time difference of 15.86 hours  
##  
## $nightlength  
## Time difference of 8.14 hours
```

As a final example, 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 24.94 60.17

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

## $day
## [1] "2013-09-21 UTC"
##
## $sunrise
## [1] "2013-09-21 07:08:45 EEST"
##
## $noon
## [1] "2013-09-21 13:12:49 EEST"
##
## $sunset
## [1] "2013-09-21 19:16:23 EEST"
##
## $daylength
## Time difference of 12.13 hours
##
## $nightlength
## Time difference of 11.87 hours

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

## $day
## [1] "2013-09-21 UTC"
##
## $sunrise
## [1] "2013-09-21 07:57:16 EEST"
##
## $noon
## [1] "2013-09-21 13:12:49 EEST"
##
## $sunset
## [1] "2013-09-21 18:28:02 EEST"
##
## $daylength
## Time difference of 10.51 hours
##
## $nightlength
## Time difference of 13.49 hours

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

## $day
## [1] "2013-09-21 UTC"
##
```

```

## $sunrise
## [1] "2013-09-21 08:47:20 EEST"
##
## $noon
## [1] "2013-09-21 13:12:49 EEST"
##
## $sunset
## [1] "2013-09-21 17:38:05 EEST"
##
## $daylength
## Time difference of 8.846 hours
##
## $nightlength
## Time difference of 15.15 hours

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

## $day
## [1] "2013-09-21 UTC"
##
## $sunrise
## [1] "2013-09-21 09:41:31 EEST"
##
## $noon
## [1] "2013-09-21 13:12:49 EEST"
##
## $sunset
## [1] "2013-09-21 16:44:00 EEST"
##
## $daylength
## Time difference of 7.041 hours
##
## $nightlength
## Time difference of 16.96 hours

```

## 7.4 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 29.76 62.6

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] 267.6
##
## $elevation
## [1] 25.82
##
## $diameter
## [1] 0.526
##
## $distance
## [1] 1.014
```

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] "2014-06-29 13:56:36 EEST"
##
## $azimuth
## [1] 198.7
##
## $elevation
## [1] 49.64
##
## $diameter
## [1] 0.5245
##
## $distance
## [1] 1.017
```

## 7.5 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)
elevations <- sun_angles(hours,
                         lon = geo_code_He[["lon"]],
                         lat = geo_code_He[["lat"]])$elevation
sun_elev_hel <- data.frame(time_eet = hours,
```

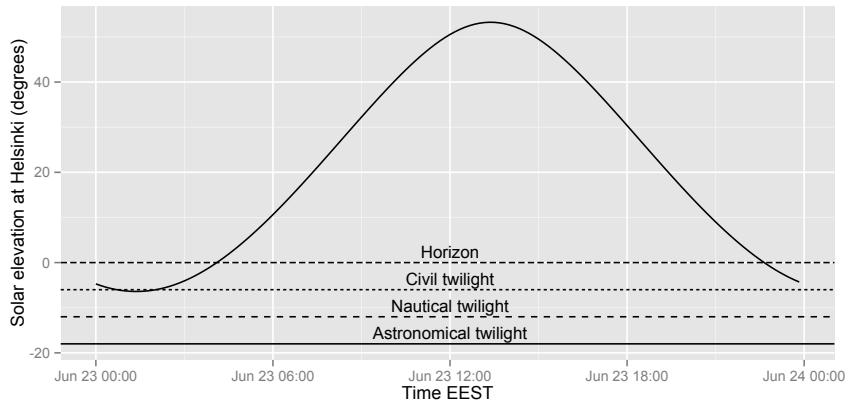
```
elevation = elevations,
location = "Helsinki",
lon = geo_code_He[["lon"]],
lat = geo_code_He[["lat"]])
```

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")
```



## 7.6 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:

```

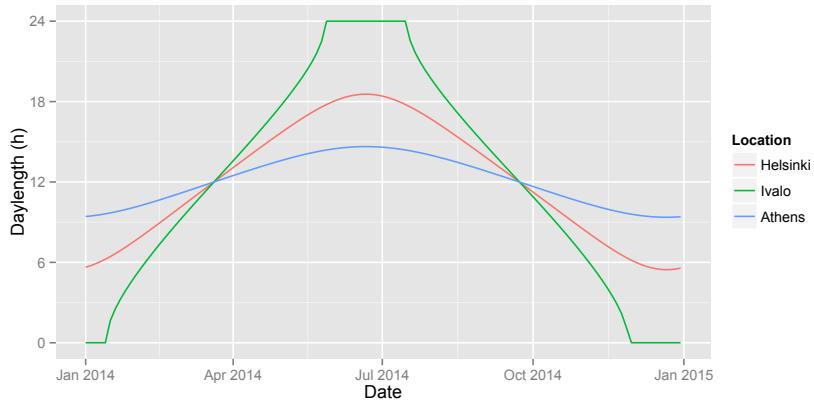
len_days <- length(days)
photoperiods <- numeric(len_days)
geo_code_He <- geocode("Helsinki")
for (i in 1:len_days) {
  day_night.ls <- day_night(days[i],
    lon = geo_code_He[["lon"]],
    lat = geo_code_He[["lat"]],
    tz="EET")
  photoperiods[i] <-
    as.numeric(day_night.ls[["daylength"]],
      units="hours")
}
daylengths_hel <-
  data.frame(day = days,
    daylength = photoperiods,
    location="Helsinki",
    lon = geo_code_He[["lon"]],
    lat = geo_code_He[["lat"]])
geo_code_Iv <- geocode("Ivalo")
for (i in 1:len_days) {
  day_night.ls <- day_night(days[i],
    lon = geo_code_Iv[["lon"]],
    lat = geo_code_Iv[["lat"]],
    tz="EET")
  photoperiods[i] <-
    as.numeric(day_night.ls[["daylength"]],
      units="hours")
}
daylengths_ivalo <-
  data.frame(day = days,
    daylength = photoperiods,
    location="Ivalo",
    lon = geo_code_Iv[["lon"]],
    lat = geo_code_Iv[["lat"]])
geo_code_At <- geocode("Athens, Greece")
for (i in 1:len_days) {
  day_night.ls <- day_night(days[i],
    lon = geo_code_At[["lon"]],
    lat = geo_code_At[["lat"]],
    tz="EET")
  photoperiods[i] <-
    as.numeric(day_night.ls[["daylength"]],
      units="hours")
}
daylengths_athens <-
  data.frame(day = days,
    daylength = photoperiods,
    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")
```





CHAPTER  
8

## Basic operations on spectra

### Abstract

In this chapter we describe the use of a few basic functions, which can be useful when no predefined functions are available for a given operation.

### 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(photobiologyFilters)
library(photobiologyLEDs)
```

### 8.2 Introduction

#### How are example spectra stored?

The suite uses to some extent object-oriented programming. Objects are implemented using “S3” classes. For spectra the classes are a specialization of `data.table` which are in turn a specialization of `data.frame`. This means that they are compatible with functions that operate on these classes.

The suite defines a “`generic.spct`” class, from which two specialized classes, “`filter.spct`” and “`source.spct`” are derived. Having this class structure allows us to create special methods and operators, which use the same names than the generic ones but take into account the special properties of spectra. Each spectrum object can hold only one spectrum.

Objects of class “`source.spct`” have three components `w.length`, `s.e.irrad` and `s.q.irrad`. They are expected to contain data expressed

always in the same units: nm, for `w.length`,  $\text{W m}^{-2} \text{nm}^{-1}$  for `s.e.irrad`, and  $\text{mol m}^{-2} \text{s}^{-1} \text{nm}^{-1}$  for `s.q.irrad`. Objects have a "comment" attribute with a textual description.

Objects of class "filter.spct" have three components `w.length`, `Tfr` and `Tpc`. They are expected to contain data expressed always in the same units: nm, for `w.length`, a fraction of one for `Tfr`, and % for `Tpc`. Objects have a "comment" attribute with a textual description.

### **What operators are available for operations between spectra?**

Operators are defined for these objects. These are an easy and simple way of doing calculations, but are rather inflexible and performance is expected to be slower than with functions with additional parameters. The operators are defined so that an operation between two "filter.spct" objects yields another "filter.spct" object, and operation between a "filter.spct" object and a "source.spct", or between two "source.spct" objects yields a "source.spct" object. 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.

### **What operators are available for operations between spectra and numeric vectors?**

The same four operators plus power (' $\wedge$ ') are defined for the case when the first term or factor is a spectrum and the second one a numeric vector, possibly of length one. Recycling rules apply. These operations do not alter `w.length`, just the other components such as spectral irradiance and transmittance.

### **What functions are available for operations between spectra?**

Logarithms (`log`, `log10`), square root (`sqrt`) and exponentiation (`exp`) are defined for spectra. These functions are not applied on `w.length`, but instead on the other components such as spectral irradiance and spectral transmittance.

### **What 'summary' functions are available for spectra?**

The R functions `summary`, `print` work in their predefined form, however, there are special versions of `range`, `min`, `max` that when applied to spectra return values corresponding to wavelengths, two generic functions defined in the suite give additional summaries of spectra `spread`, `midpoint`.

### **Examples**

Package `phobiologyFilters` 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<sup>1</sup>.

```
filtered_sun.dt <- sun.dt * gg400.dt
head(filtered_sun.dt)

##      w.length s.e.irrad s.q.irrad
## 1:      293 2.610e-11 6.392e-17
## 2:      294 6.142e-11 1.510e-16
## 3:      295 2.176e-10 5.366e-16
## 4:      296 6.780e-10 1.678e-15
## 5:      297 1.533e-09 3.807e-15
## 6:      298 3.670e-09 9.141e-15
```

The GG440 data is for internal transmittance. Let's assume a filter with 9% reflection across all wavelengths (a coarse approximation):

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

##      w.length s.e.irrad s.q.irrad
## 1:      293 2.375e-11 5.816e-17
## 2:      294 5.590e-11 1.374e-16
## 3:      295 1.980e-10 4.883e-16
## 4:      296 6.170e-10 1.527e-15
## 5:      297 1.395e-09 3.465e-15
## 6:      298 3.339e-09 8.319e-15
```

Calculations related to filters will be explained in detail in chapter 15. This is just an example of how the operators work.

### 8.3 Task: uniform scaling of a spectrum

As noted above operators are available for "generic.scpt", "source.sptc", and "filter.sptc" objects, and 'recycling' takes places when needed:

```
head(sun.dt)

##      w.length s.e.irrad s.q.irrad
## 1:      293 2.610e-06 6.392e-12
## 2:      294 6.142e-06 1.510e-11
## 3:      295 2.176e-05 5.366e-11
## 4:      296 6.780e-05 1.678e-10
## 5:      297 1.533e-04 3.807e-10
## 6:      298 3.670e-04 9.141e-10

head(sun.dt * 2)

##      w.length s.e.irrad s.q.irrad
## 1:      293 5.219e-06 1.278e-11
## 2:      294 1.228e-05 3.019e-11
## 3:      295 4.352e-05 1.073e-10
## 4:      296 1.356e-04 3.355e-10
## 5:      297 3.067e-04 7.614e-10
## 6:      298 7.339e-04 1.828e-09
```

---

<sup>1</sup>Here and in many other examples `head` is used to limit the amount of output to a few lines.

All four basic binary operators (+, -, \*, /) can be used in the same way, but when operating between a spectrum an a numeric value the spectrum should be the first term or factor. If an operation on a “source.spct” would yield different values for data on energy and photon basis, only the value based on energy data is returned in `s.e.irrad` and `s.q.irrad` is set to NA.

## 8.4 Task: simple operations between two spectra

```
filtered_sun.dt <- ug1.dt * sun.dt
head(filtered_sun.dt)

##      w.length s.e.irrad s.q.irrad
## 1:      293 2.286e-07 5.599e-13
## 2:      294 6.192e-07 1.522e-12
## 3:      295 2.481e-06 6.118e-12
## 4:      296 8.624e-06 2.134e-11
## 5:      297 2.153e-05 5.345e-11
## 6:      298 5.637e-05 1.404e-10
```

All four basic binary operators (+, -, \*, /) can be used in the same way.

## 8.5 Task: other operations between two spectra

If data for two spectra are available for the same wavelength values, then we can still use the built in R mat operators. These operators are vectorized, which means that an addition between two vectors adds the elements at each position. A non-nonsensical example follows:

```
head(with(sun.data, s.e.irrad^2 / w.length))

## [1] 2.324e-14 1.283e-13 1.605e-12 1.553e-11
## [5] 7.918e-11 4.519e-10
```

Operations using built-in R operators cannot be done if the wavelengths in two spectral data sets do not match. In this situation is where functions 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). The functions are `sum_spectra`, `subt_spectra`, `prod_spectra`, `div_spectra`, and `oper_spectra`. Here is a very simple hypothetical example:

```
out1.dt <- sum_spectra(spc1$w.length, spc2$w.length,
                        spc1$s.e.irrad, spc2$s.e.irrad)
```

This is what happens under the hood when we execute code like:

```
out2.data <- spc1 + spc2
```

with the difference that in the first case only spectral energy irradiance is calculated, while in the second both spectral energy irradiance and spectral

photon irradiance are returned. `out1.data` is a "data.table", while the second will be an spectrum of a class dependent on the classes of `spc1` and `spc2`. Obviously, the second calculation will be slower, but in most cases unnoticeable so.

The function `oper_spectra` takes the operator to use as an argument:

```
out.data <- oper_spectra(spc1$w.length, spc2$w.length,
                           spc1$s.e.irrad, spc2$s.e.irrad,
                           bin.oper='^`')
```

and yields the 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.

## 8.6 Task: trimming a spectrum

This is basically a subsetting operation, but the function `trim_tails` adds a few 'bells and whistles'. The trimming is based on wavelengths, by default the cut points are inserted by interpolation, so that the spectrum returned includes the limits given as arguments. By default the trimming is done by deleting both spectral irradiance and wavelength values outside the range delimited by the limits, but through parameter `fill` the values outside the limits can be replaced any value desired (most commonly NA or 0.) It is possible to supply only one, or both of `low.limit` and `high.limit`, depending on the desired trimming.

```
head(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                     low.limit=300)))

##   w.length  s.irrad
## 1      300 0.001265
## 2      301 0.002624
## 3      302 0.003923
## 4      303 0.008974
## 5      304 0.011656
## 6      305 0.017991

head(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                     low.limit=300, fill=NULL)))

##   w.length  s.irrad
## 1      300 0.001265
## 2      301 0.002624
## 3      302 0.003923
## 4      303 0.008974
## 5      304 0.011656
## 6      305 0.017991

head(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                     low.limit=300, fill=NA)))
```

```

##      w.length s.irrad
## 1      293     NA
## 2      294     NA
## 3      295     NA
## 4      296     NA
## 5      297     NA
## 6      298     NA

head(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                      low.limit=300, fill=0.0)))

##      w.length s.irrad
## 1      293      0
## 2      294      0
## 3      295      0
## 4      296      0
## 5      297      0
## 6      298      0

```

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.

```

tail(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                      low.limit=300, high.limit=1000)))

## Warning: Ignoring high.limit as it is too high.

##      w.length s.irrad
## 496      795  0.4147
## 497      796  0.4081
## 498      797  0.4141
## 499      798  0.4236
## 500      799  0.4186
## 501      800  0.4069

tail(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                      low.limit=300, high.limit=1000, fill=NA)))

##      w.length s.irrad
## 703      995     NA
## 704      996     NA
## 705      997     NA
## 706      998     NA
## 707      999     NA
## 708     1000     NA

tail(with(sun.data,
          trim_tails(w.length, s.e.irrad,
                      low.limit=300, high.limit=1000, fill=0.0)))

##      w.length s.irrad
## 703      995      0
## 704      996      0
## 705      997      0
## 706      998      0
## 707      999      0
## 708     1000      0

```

## 8.7 Task: conversion from energy to photon base

The energy of a quantum of radiation in a vacuum,  $q$ , depends on the wavelength,  $\lambda$ , or frequency<sup>2</sup>,  $\nu$ ,

$$q = h \cdot \nu = h \cdot \frac{c}{\lambda} \quad (8.1)$$

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<sup>-1</sup>. When dealing with numbers of photons, the equation (8.1) can be extended by using Avogadro's number  $N_A = 6.022 \times 10^{23}$  mol<sup>-1</sup>. Thus, the energy of one mole of photons,  $q'$ , is

$$q' = h' \cdot \nu = h' \cdot \frac{c}{\lambda} \quad (8.2)$$

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

Function `as_quantum` converts W m<sup>-2</sup> into *number of photons* per square meter per second, and `as_quantum_mol` does the same conversion but returns mol m<sup>-2</sup> s<sup>-1</sup>. Function `as_quantum` is based on the equation 8.1 while `as_quantum_mol` uses equation 8.2. To obtain μmol m<sup>-2</sup> s<sup>-1</sup> we multiply by 10<sup>6</sup>:

```
as_quantum_mol(550, 200) * 1e6
## [1] 919.5
```

The calculation above is for monochromatic light (200 W m<sup>-2</sup> at 550 nm).

The functions are vectorized, so they can be applied to whole spectra, to convert W m<sup>-2</sup> nm<sup>-1</sup> to mol m<sup>-2</sup> s<sup>-1</sup> nm<sup>-1</sup>:

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

## [1] 2.610e-06 6.142e-06 2.176e-05 6.780e-05
## [5] 1.533e-04 3.670e-04 7.845e-04 1.265e-03
## [9] 2.624e-03 3.923e-03

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

## [1] 6.392e-12 1.510e-11 5.366e-11 1.678e-10
## [5] 3.807e-10 9.141e-10 1.961e-09 3.171e-09
## [9] 6.602e-09 9.903e-09
```

## 8.8 Task: conversion from photon to energy base

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

In `aphalo2012` it is written: “Example 1: red light at 600 nm has about 200 kJ mol<sup>-1</sup>, therefore, 1 μmol photons has 0.2 J. Example 2: UV-B radiation at

---

<sup>2</sup>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 8.1.

300 nm has about 400  $\text{kJ mol}^{-1}$ , therefore, 1  $\mu\text{mol}$  photons has 0.4 J. Equations 8.1 and 8.2 are valid for all kinds of electromagnetic waves.” Let’s re-calculate the exact values—as the output is we multiply by  $10^{-3}$  to obtain  $\text{kJ mol}^{-1}$ :

```
as_energy(600, 1) * 1e-3
## [1] 199.4
as_energy(300, 1) * 1e-3
## [1] 398.8
```

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

```
head(sun.data$s.q.irrad, 10)
## [1] 6.392e-12 1.510e-11 5.366e-11 1.678e-10
## [5] 3.807e-10 9.141e-10 1.961e-09 3.171e-09
## [9] 6.602e-09 9.903e-09

s.e.irrad <- with(sun.data, as_energy(w.length, s.q.irrad))
head(s.e.irrad, 10)
## [1] 2.610e-06 6.142e-06 2.176e-05 6.780e-05
## [5] 1.533e-04 3.670e-04 7.845e-04 1.265e-03
## [9] 2.624e-03 3.923e-03
```

## 8.9 Task: interpolating a spectrum

The function `interpolate_spectrum` is used internally for interpolating spectra, 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 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`:

```
with(sun.data,
     interpolate_spectrum(w.length, s.e.irrad, 290:300))

## [1] NA NA NA 2.610e-06
## [5] 6.142e-06 2.176e-05 6.780e-05 1.533e-04
## [9] 3.670e-04 7.845e-04 1.265e-03

with(sun.data,
     interpolate_spectrum(w.length, s.e.irrad, 290:300, fill=0.0))

## [1] 0.000e+00 0.000e+00 0.000e+00 2.610e-06
## [5] 6.142e-06 2.176e-05 6.780e-05 1.533e-04
## [9] 3.670e-04 7.845e-04 1.265e-03
```

This function, in its current implementation, always returns interpolated values, even when the density of wavelengths in the output is less than that in the input. A future version will *likely* include a parameter for changing this behaviour to averaging or smoothing.

## 8.10 Internal-use functions

The function `check_spectrum` may need to be called by the user if he/she disables automatic sanity checking to increase calculation speed. The family of functions for calculating multipliers are used internally by the package.

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

The function `integrate_irradiance` is used internally for integrating spectra, 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, or never. This function makes it possible to work with spectral data on the original pixel wavelengths.



CHAPTER



## Unweighted irradiance

### Abstract

In this chapter we explain how to calculate unweighted energy and photon irradiances from spectral irradiance.

### 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(photobiologyVIS)
library(photobiologyUV)
```

### 9.2 Introduction

### 9.3 Task: (energy) irradiance from spectral irradiance

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

$$E_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda) \, d\lambda \quad (9.1)$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) energy irradiance, for which the most accepted limits are  $\lambda_1 = 400\text{nm}$  and  $\lambda_2 = 700\text{nm}$ . In this example we will use example data for sunlight to calculate  $E_{400\text{nm} < \lambda < 700\text{nm}}$ :

```
with(sun.data,
      energy_irradiance(w.length, s.e.irrad,
                          new_waveband(400, 700)))

## range.400.700
##           196.7
```

Function PAR() is predefined in package photobiologyVIS as a convenience function, so the code above can be replaced by:

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

##    PAR
## 196.7
```

If no waveband is supplied as argument, then the whole range of wavelengths in the spectral data is used for the integration, and the ‘name’ attribute is generated accordingly:

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

## range.293.800
##          269.1
```

If a waveband that does not fully overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

```
with(sun.data,
      energy_irradiance(w.length, s.e.irrad,
                          new_waveband(700, 1000)))

## range.700.1000
##           44.1
```

If a waveband that does not overlap with the data is supplied as argument, then spectral irradiance for wavelengths outside the range is assumed to be zero:

```
with(sun.data,
      energy_irradiance(w.length, s.e.irrad,
                          new_waveband(100, 200)))

## range.100.200
##            0
```

## 9.4 Task: photon irradiance from spectral irradiance

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

Combining equations 9.1 and 8.2 we obtain:

$$Q_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} E(\lambda) \frac{h' \cdot c}{\lambda} d\lambda \quad (9.2)$$

Let's assume that we want to calculate photosynthetically active radiation (PAR) photon irradiance. In this example we will use example data for sunlight.

```
with(sun.data,
  photon_irradiance(w.length, s.e.irrad, PAR()))

##      PAR
## 0.0008938
```

If we want to have  $Q_{\text{PAR}}$  (PPFD) expressed in the usual units of  $\mu\text{mol m}^{-2} \text{s}^{-1}$ , we need to multiply the result above by  $10^6$ :

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

##      PAR
## 893.8
```

`PAR()` is predefined in package `photobiologyVIS` as a convenience function, see section ?? for an example with arbitrary values for  $\lambda_1$  and  $\lambda_2$ .

## 9.5 Task: calculate energy and photon irradiances from spectral photon irradiance

In the case of the calculation of energy irradiance from spectral photon irradiance the calculation is:

$$E_{\lambda_1 < \lambda < \lambda_2} = \int_{\lambda_1}^{\lambda_2} Q(\lambda) \frac{\lambda}{h' \cdot c} d\lambda \quad (9.3)$$

And the code<sup>1</sup>:

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

##      PAR
## 0.0008938
```

The calculation of photon irradiance from spectral photon irradiance, is a simple integration, analogous to that in equation 9.1, and the code is:

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

##      PAR
## 4.158e-09
```

---

<sup>1</sup>The dataframe `sun.data` contains both spectral energy irradiance values in 'column' `s.e.irrad` and spectral photon irradiance in 'column' `s.q.irrad`

## 9.6 Task: irradiances for more than one waveband

It is possible to calculate the irradiances for several wavebands with a single function call by supplying a list of wavebands as argument:

```
with(sun.data,
      photon_irradiance(w.length, s.e.irrad,
                          list(Red(), Green(), Blue()))) * 1e6

##     Red.ISO Green.ISO  Blue.ISO
##     452.2      220.2      149.0

Q.RGB <- with(sun.data,
      photon_irradiance(w.length, s.e.irrad,
                          list(Red(), Green(), Blue()))) * 1e6
signif(Q.RGB, 3)

##     Red.ISO Green.ISO  Blue.ISO
##     452       220       149

Q.RGB[1]

## Red.ISO
## 452.2

Q.RGB["Green.ISO"]

## Green.ISO
## 220.2
```

A named list can be used to override the use as names for the output of the waveband names:

```
with(sun.data,
      photon_irradiance(w.length, s.e.irrad,
                          list(R=Red(), G=Green(), B=Blue()))) * 1e6

##     R      G      B
## 452.2 220.2 149.0
```

Even when using a single waveband:

```
with(sun.data,
      photon_irradiance(w.length, s.e.irrad,
                          list(UVB=UVB())))) * 1e6

##    UVB
## 1.527
```

## 9.7 Task: use simple wavebands

Please, consult the packages' documentation for a list of predefined functions for creating wavebands. 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 49

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
```

As seen above, there is a specialized `print` function for wavebands. Functions available are `min`, `max`, `range`, `center_wl`, `labels`, and `color`.

```
red <- Red()
red

## Red.ISO
## low (nm) 610
## high (nm) 760

min(red)
## [1] 610

max(red)
## [1] 760

range(red)
## [1] 610 760

midpoint(red)
## [1] 685

labels(red)

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

color(red)

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

Here we demonstrate the use of an argument to choose a certain definition:

```
UVB()

## UVB.ISO
```

```

## low (nm) 280
## high (nm) 315

UVB("ISO")

## UVB.ISO
## low (nm) 280
## high (nm) 315

UVB("CIE")

## UVB.CIE
## low (nm) 280
## high (nm) 315

UVB("medical")

## UVB.medical
## low (nm) 290
## high (nm) 320

UVB("none")

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

```

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

```

with(sun.data,
      photon_irradiance(w.length, s.e.irrad, UVB("ISO")) * 1e6

## UVB.ISO
##     1.527

with(sun.data,
      photon_irradiance(w.length, s.e.irrad, UVB("none")) * 1e6

## UVB.none
##     3.282

```

## 9.8 Task: define simple wavebands

Here we briefly introduce **new\_waveband**, and only in chapter ?? we describe its use in full detail, including the use of spectral weighting functions (SWFs). Defining a new **waveband** based on extreme wavelengths expressed in nm.

```

wb1 <- new_waveband(500,600)
wb1

## range.500.600
## low (nm) 500
## high (nm) 600

```

```

with(sun.data,
  photon_irradiance(w.length, s.e.irrad, wb1)) * 1e6

## range.500.600
##           314.1

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

## my.colour
## low (nm) 500
## high (nm) 600

with(sun.data,
  photon_irradiance(w.length, s.e.irrad, wb2)) * 1e6

## my.colour
##           314.1

```

## 9.9 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  $\zeta$ ). If we follow the wavelength ranges in the definition given by **Morgan1981a** using photon irradiance<sup>2</sup>:

$$\zeta = \frac{Q_{655\text{nm} < \lambda < 665\text{nm}}}{Q_{725\text{nm} < \lambda < 735\text{nm}}} \quad (9.4)$$

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

```

with(sun.data,
  photon_ratio(w.length, s.e.irrad,
    Red("Smith"), Far_red("Smith")))

## [1] 1.251

```

or using the predefined convenience function **R\_FR\_ratio**:

```

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

## [1] 1.251

```

Using defaults for waveband definitions:

---

<sup>2</sup>In the original text photon fluence rate is used but it not clear whether photon irradiance was meant instead.

```
with(sun.data,
      energy_ratio(w.length, s.e.irrad, UVB(), PAR()))

## [1] 0.00299
```

## 9.10 Task: energy ratios

An energy ratio, equivalent to  $\zeta$  can be calculated as follows:

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

## [1] 1.384
```

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

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

$$\bar{q}' = \frac{Q_{\lambda_1 < \lambda < \lambda_2}}{E_{\lambda_1 < \lambda < \lambda_2}} \quad (9.5)$$

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

## [1] 4.544e-06
```

For obtaining the same quotient in  $\mu\text{mol J}^{-1}$  we just need to multiply by  $10^6$ . We can use such a multiplier to convert  $E [\text{W m}^{-2}]$  into  $Q [\mu\text{mol m}^{-2} \text{s}^{-1}]$  (as  $\text{W} = \text{Js}^{-1}$ ), or as a divisor to convert  $Q [\mu\text{mol m}^{-2} \text{s}^{-1}]$  into  $E [\text{W m}^{-2}]$ , *for a given light source and waveband*:

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

## [1] 4.544
```

## 9.12 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. We can use the function `split_energy_irradiance` to obtain to energy of each of the regions delimited by the values in nm supplied in a numeric vector:



```
## range.400.500 range.500.600
##          50.4           49.6
```

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

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

## range.400.700
##          196.7
```

### 9.13 Task: calculate the contribution of different regions of a spectrum to photon irradiance

The function `split_photon_irradiance` takes the same arguments as the equivalent function for photon irradiance, consequently only one code example is provided here (see section 9.12 for more details):

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

## range.400.500 range.500.600 range.600.700
##          29.41           35.14           35.45
```

# CHAPTER 10

## Weighted and effective irradiance

### Abstract

In this chapter we explain how to calculate weighted 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(photobiologyVIS)
library(photobiologyUV)
```

### 10.2 Introduction

Weighted irradiance is usually reported in weighted energy units, but it is possible to also 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 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 use a biological spectral weighting function (BSWF). The focus of this chapter is on the differences between calculations for weighted irradiances compared to those for unweighted irradiances described in chapter 9. In particular it is important that you read sections 9.3, 9.4, ??, and 9.6 before reading the present chapter.

### 10.3 Task: choosing the normalization wavelength

Function `GEN.G()` is predefined in package `photobiologyUV` as a convenience function for Green's formulation of Caldwell's generalized plant action spectrum (GPAS) `Green198x`

```
with(sun.data,
  energy_irradiance(w.length, s.e.irrad, GEN.G()))

## GEN.G.300
##      0.1034
```

The code above uses the default normalization wavelength of 300 nm. Any arbitrary wavelength (nm), within the range of the waveband can be provided as an argument.

```
range(GEN.G())
## [1] 250.0 313.3

with(sun.data,
  energy_irradiance(w.length, s.e.irrad, GEN.G(280)))

## GEN.G.280
##      0.02402
```

### 10.4 Task: use weighted wavebands

Please, consult the packages' documentation for a list of predefined functions for creating weighted wavebands. Here we will present just a few examples of their use. We usually think of weighted irradiances as being defined by the weighting function, however, in many cases different normalizations are in use, and the result of any calculation depends very strongly on the wavelength used for normalization. For this reason, the functions provided accept an argument that can be used to select the normalization wavelength. In general, the default, is to use the most frequently used normalization.

In a few cases different mathematical formulations are available for the same spectrum, and the differences among them can be quite large. In such cases separate functions are provided for each of them (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) 250
## high (nm) 313
## weighted SWF
## normalized at 300 nm

GEN.G(300)
```

```
## GEN.G.300
## low (nm) 250
## high (nm) 313
## weighted SWF
## normalized at 300 nm

GEN.G(280)

## GEN.G.280
## low (nm) 250
## high (nm) 313
## weighted SWF
## normalized at 280 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 seen above, there is a specialized `print` function for wavebands. Functions available are `min`, `max`, `range`, `midpoint`, `labels`, and `color`.

```
min(cie)
## [1] 250
max(cie)
## [1] 400
range(cie)
## [1] 250 400
midpoint(cie)
## [1] 325
normalization(cie)
## [1] 298
labels(cie)
## $label
## [1] "CIE98"
##
## $name
## [1] "CIE98.298"
color(cie)
## CIE98 CMF CIE98 CC
## "#02000F" "#1A00DD"
```

## 10.5 Task: define wavebands

In section ?? we briefly introduced `new_waveband`, and here we describe its use in full detail, including the use of spectral weighting functions (SWFs).

Defining a new weighted waveband. We start with a simple ‘toy’ example:

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

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

with(sun.data,
      energy_irradiance(w.length, s.e.irrad, toy.wb))

##      TOY
## 241.7

with(sun.data,
      photon_irradiance(w.length, s.e.irrad, toy.wb))

##      TOY
## 0.001111
```

## 10.6 Introduction

## Transmission and reflection

### Abstract

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

### 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(photobiologyFilters)
```

### 11.2 Introduction

### 11.3 Task: absorbance and transmittance

Transmittance is defined as:

$$\tau(\lambda) = \frac{I}{I_0} = \frac{E(\lambda)}{E_0(\lambda)} = \frac{Q(\lambda)}{Q_0(\lambda)} \quad (11.1)$$

Given this simple relation  $\tau(\lambda)$  can be calculated as a division between two "source.spc" 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:

$$A(\lambda) = -\log_{10} \frac{I}{I_0} \quad (11.2)$$

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:

$$A(\lambda) = -\log_{10} \tau(\lambda) \quad (11.3)$$

which in S language is:

```
T2A <- function(x) {-log10(x)}
```

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

$$\tau(\lambda) = 10^{-A(\lambda)} \quad (11.4)$$

which in S language is:

```
A2T <- function(x) {10^x}
```

They could be directly applied to spectra but doing this still gives "filter.spc" objects as a result, with the data labelled "T", when it has changed into absorbance. 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.ggg400.dt <- copy(gg400.dt)
my.ggg400.dt[, A := T2A(Tfr)]

##      w.length    Tfr     Tpc   A
## 1:      200 1e-05 0.001 5
## 2:      210 1e-05 0.001 5
## 3:      220 1e-05 0.001 5
## 4:      230 1e-05 0.001 5
## 5:      240 1e-05 0.001 5
## 6:      250 1e-05 0.001 5
## 7:      260 1e-05 0.001 5
## 8:      270 1e-05 0.001 5
## 9:      280 1e-05 0.001 5
## 10:     290 1e-05 0.001 5
## 11:     300 1e-05 0.001 5
## 12:     310 1e-05 0.001 5
## 13:     320 1e-05 0.001 5
## 14:     330 1e-05 0.001 5
## 15:     340 1e-05 0.001 5
## 16:     350 1e-05 0.001 5
## 17:     360 1e-05 0.001 5
## 18:     370 1e-05 0.001 5
## 19:     380 1e-05 0.001 5
## 20:     390 1e-05 0.001 5
## 21:     400 1e-05 0.001 5
## 22:     410 1e-05 0.001 5
## 23:     420 1e-05 0.001 5
## 24:     430 1e-05 0.001 5
## 25:     440 1e-05 0.001 5
## 26:     450 1e-05 0.001 5
## 27:     460 1e-05 0.001 5
## 28:     470 1e-05 0.001 5
## 29:     480 1e-05 0.001 5
## 30:     490 1e-05 0.001 5
## 31:     500 1e-05 0.001 5
## 32:     510 1e-05 0.001 5
## 33:     520 1e-05 0.001 5
## 34:     530 1e-05 0.001 5
## 35:     540 1e-05 0.001 5
## 36:     550 1e-05 0.001 5
## 37:     560 1e-05 0.001 5
## 38:     570 1e-05 0.001 5
## 39:     580 1e-05 0.001 5
## 40:     590 1e-05 0.001 5
## 41:     600 1e-05 0.001 5
## 42:     610 1e-05 0.001 5
## 43:     620 1e-05 0.001 5
## 44:     630 1e-05 0.001 5
## 45:     640 1e-05 0.001 5
## 46:     650 1e-05 0.001 5
## 47:     660 1e-05 0.001 5
## 48:     670 1e-05 0.001 5
## 49:     680 1e-05 0.001 5
## 50:     690 1e-05 0.001 5
## 51:     700 1e-05 0.001 5
## 52:     710 1e-05 0.001 5
## 53:     720 1e-05 0.001 5
## 54:     730 1e-05 0.001 5
## 55:     740 1e-05 0.001 5
## 56:     750 1e-05 0.001 5
## 57:     760 1e-05 0.001 5
## 58:     770 1e-05 0.001 5
## 59:     780 1e-05 0.001 5
## 60:     790 1e-05 0.001 5
## 61:     800 1e-05 0.001 5
## 62:     810 1e-05 0.001 5
## 63:     820 1e-05 0.001 5
## 64:     830 1e-05 0.001 5
## 65:     840 1e-05 0.001 5
## 66:     850 1e-05 0.001 5
## 67:     860 1e-05 0.001 5
## 68:     870 1e-05 0.001 5
## 69:     880 1e-05 0.001 5
## 70:     890 1e-05 0.001 5
## 71:     900 1e-05 0.001 5
## 72:     910 1e-05 0.001 5
## 73:     920 1e-05 0.001 5
## 74:     930 1e-05 0.001 5
## 75:     940 1e-05 0.001 5
## 76:     950 1e-05 0.001 5
## 77:     960 1e-05 0.001 5
## 78:     970 1e-05 0.001 5
## 79:     980 1e-05 0.001 5
## 80:     990 1e-05 0.001 5
## 81:     1000 1e-05 0.001 5
## 82:     1010 1e-05 0.001 5
## 83:     1020 1e-05 0.001 5
## 84:     1030 1e-05 0.001 5
## 85:     1040 1e-05 0.001 5
## 86:     1050 1e-05 0.001 5
## 87:     1060 1e-05 0.001 5
## 88:     1070 1e-05 0.001 5
## 89:     1080 1e-05 0.001 5
## 90:     1090 1e-05 0.001 5
## 91:     1100 1e-05 0.001 5
## 92:     1110 1e-05 0.001 5
## 93:     1120 1e-05 0.001 5
## 94:     1130 1e-05 0.001 5
## 95:     1140 1e-05 0.001 5
## 96:     1150 1e-05 0.001 5
## 97:     1160 1e-05 0.001 5
## 98:     1170 1e-05 0.001 5
## 99:     1180 1e-05 0.001 5
## 100:    1190 1e-05 0.001 5
## 101:    1200 1e-05 0.001 5
## 102:    1210 1e-05 0.001 5
## 103:    1220 1e-05 0.001 5
## 104:    1230 1e-05 0.001 5
## 105:    1240 1e-05 0.001 5
## 106:    1250 1e-05 0.001 5
## 107:    1260 1e-05 0.001 5
## 108:    1270 1e-05 0.001 5
## 109:    1280 1e-05 0.001 5
## 110:    1290 1e-05 0.001 5
## 111:    1300 1e-05 0.001 5
## 112:    1310 1e-05 0.001 5
## 113:    1320 1e-05 0.001 5
## 114:    1330 1e-05 0.001 5
## 115:    1340 1e-05 0.001 5
## 116:    1350 1e-05 0.001 5
## 117:    1360 1e-05 0.001 5
## 118:    1370 1e-05 0.001 5
## 119:    1380 1e-05 0.001 5
## 120:    1390 1e-05 0.001 5
## 121:    1400 1e-05 0.001 5
## 122:    1410 1e-05 0.001 5
## 123:    1420 1e-05 0.001 5
## 124:    1430 1e-05 0.001 5
## 125:    1440 1e-05 0.001 5
## 126:    1450 1e-05 0.001 5
## 127:    1460 1e-05 0.001 5
## 128:    1470 1e-05 0.001 5
## 129:    1480 1e-05 0.001 5
## 130:    1490 1e-05 0.001 5
## 131:    1500 1e-05 0.001 5
## 132:    1510 1e-05 0.001 5
## 133:    1520 1e-05 0.001 5
## 134:    1530 1e-05 0.001 5
## 135:    1540 1e-05 0.001 5
## 136:    1550 1e-05 0.001 5
## 137:    1560 1e-05 0.001 5
## 138:    1570 1e-05 0.001 5
## 139:    1580 1e-05 0.001 5
## 140:    1590 1e-05 0.001 5
## 141:    1600 1e-05 0.001 5
## 142:    1610 1e-05 0.001 5
## 143:    1620 1e-05 0.001 5
## 144:    1630 1e-05 0.001 5
## 145:    1640 1e-05 0.001 5
## 146:    1650 1e-05 0.001 5
## 147:    1660 1e-05 0.001 5
## 148:    1670 1e-05 0.001 5
## 149:    1680 1e-05 0.001 5
## 150:    1690 1e-05 0.001 5
## 151:    1700 1e-05 0.001 5
## 152:    1710 1e-05 0.001 5
## 153:    1720 1e-05 0.001 5
## 154:    1730 1e-05 0.001 5
## 155:    1740 1e-05 0.001 5
## 156:    1750 1e-05 0.001 5
## 157:    1760 1e-05 0.001 5
## 158:    1770 1e-05 0.001 5
## 159:    1780 1e-05 0.001 5
## 160:    1790 1e-05 0.001 5
## 161:    1800 1e-05 0.001 5
## 162:    1810 1e-05 0.001 5
## 163:    1820 1e-05 0.001 5
## 164:    1830 1e-05 0.001 5
## 165:    1840 1e-05 0.001 5
## 166:    1850 1e-05 0.001 5
## 167:    1860 1e-05 0.001 5
## 168:    1870 1e-05 0.001 5
## 169:    1880 1e-05 0.001 5
## 170:    1890 1e-05 0.001 5
## 171:    1900 1e-05 0.001 5
## 172:    1910 1e-05 0.001 5
## 173:    1920 1e-05 0.001 5
## 174:    1930 1e-05 0.001 5
## 175:    1940 1e-05 0.001 5
## 176:    1950 1e-05 0.001 5
## 177:    1960 1e-05 0.001 5
## 178:    1970 1e-05 0.001 5
## 179:    1980 1e-05 0.001 5
## 180:    1990 1e-05 0.001 5
## 181:    2000 1e-05 0.001 5
## 182:    2010 1e-05 0.001 5
## 183:    2020 1e-05 0.001 5
## 184:    2030 1e-05 0.001 5
## 185:    2040 1e-05 0.001 5
## 186:    2050 1e-05 0.001 5
## 187:    2060 1e-05 0.001 5
## 188:    2070 1e-05 0.001 5
## 189:    2080 1e-05 0.001 5
## 190:    2090 1e-05 0.001 5
## 191:    2100 1e-05 0.001 5
## 192:    2110 1e-05 0.001 5
## 193:    2120 1e-05 0.001 5
## 194:    2130 1e-05 0.001 5
## 195:    2140 1e-05 0.001 5
## 196:    2150 1e-05 0.001 5
## 197:    2160 1e-05 0.001 5
## 198:    2170 1e-05 0.001 5
## 199:    2180 1e-05 0.001 5
## 200:    2190 1e-05 0.001 5
## 201:    2200 1e-05 0.001 5
## 202:    2210 1e-05 0.001 5
## 203:    2220 1e-05 0.001 5
## 204:    2230 1e-05 0.001 5
## 205:    2240 1e-05 0.001 5
## 206:    2250 1e-05 0.001 5
## 207:    2260 1e-05 0.001 5
## 208:    2270 1e-05 0.001 5
## 209:    2280 1e-05 0.001 5
## 210:    2290 1e-05 0.001 5
## 211:    2300 1e-05 0.001 5
## 212:    2310 1e-05 0.001 5
## 213:    2320 1e-05 0.001 5
## 214:    2330 1e-05 0.001 5
## 215:    2340 1e-05 0.001 5
## 216:    2350 1e-05 0.001 5
## 217:    2360 1e-05 0.001 5
## 218:    2370 1e-05 0.001 5
## 219:    2380 1e-05 0.001 5
## 220:    2390 1e-05 0.001 5
## 221:    2400 1e-05 0.001 5
## 222:    2410 1e-05 0.001 5
## 223:    2420 1e-05 0.001 5
## 224:    2430 1e-05 0.001 5
## 225:    2440 1e-05 0.001 5
## 226:    2450 1e-05 0.001 5
## 227:    2460 1e-05 0.001 5
## 228:    2470 1e-05 0.001 5
## 229:    2480 1e-05 0.001 5
## 230:    2490 1e-05 0.001 5
## 231:    2500 1e-05 0.001 5
## 232:    2510 1e-05 0.001 5
## 233:    2520 1e-05 0.001 5
## 234:    2530 1e-05 0.001 5
## 235:    2540 1e-05 0.001 5
## 236:    2550 1e-05 0.001 5
## 237:    2560 1e-05 0.001 5
## 238:    2570 1e-05 0.001 5
## 239:    2580 1e-05 0.001 5
## 240:    2590 1e-05 0.001 5
## 241:    2600 1e-05 0.001 5
## 242:    2610 1e-05 0.001 5
## 243:    2620 1e-05 0.001 5
## 244:    2630 1e-05 0.001 5
## 245:    2640 1e-05 0.001 5
## 246:    2650 1e-05 0.001 5
## 247:    2660 1e-05 0.001 5
## 248:    2670 1e-05 0.001 5
## 249:    2680 1e-05 0.001 5
## 250:    2690 1e-05 0.001 5
## 251:    2700 1e-05 0.001 5
## 252:    2710 1e-05 0.001 5
## 253:    2720 1e-05 0.001 5
## 254:    2730 1e-05 0.001 5
## 255:    2740 1e-05 0.001 5
## 256:    2750 1e-05 0.001 5
## 257:    2760 1e-05 0.001 5
## 258:    2770 1e-05 0.001 5
## 259:    2780 1e-05 0.001 5
## 260:    2790 1e-05 0.001 5
## 261:    2800 1e-05 0.001 5
## 262:    2810 1e-05 0.001 5
## 263:    2820 1e-05 0.001 5
## 264:    2830 1e-05 0.001 5
## 265:    2840 1e-05 0.001 5
## 266:    2850 1e-05 0.001 5
## 267:    2860 1e-05 0.001 5
## 268:    2870 1e-05 0.001 5
## 269:    2880 1e-05 0.001 5
## 270:    2890 1e-05 0.001 5
## 271:    2900 1e-05 0.001 5
## 272:    2910 1e-05 0.001 5
## 273:    2920 1e-05 0.001 5
## 274:    2930 1e-05 0.001 5
## 275:    2940 1e-05 0.001 5
## 276:    2950 1e-05 0.001 5
## 277:    2960 1e-05 0.001 5
## 278:    2970 1e-05 0.001 5
## 279:    2980 1e-05 0.001 5
## 280:    2990 1e-05 0.001 5
## 281:    3000 1e-05 0.001 5
## 282:    3010 1e-05 0.001 5
## 283:    3020 1e-05 0.001 5
## 284:    3030 1e-05 0.001 5
## 285:    3040 1e-05 0.001 5
## 286:    3050 1e-05 0.001 5
## 287:    3060 1e-05 0.001 5
## 288:    3070 1e-05 0.001 5
## 289:    3080 1e-05 0.001 5
## 290:    3090 1e-05 0.001 5
## 291:    3100 1e-05 0.001 5
## 292:    3110 1e-05 0.001 5
## 293:    3120 1e-05 0.001 5
## 294:    3130 1e-05 0.001 5
## 295:    3140 1e-05 0.001 5
## 296:    3150 1e-05 0.001 5
## 297:    3160 1e-05 0.001 5
## 298:    3170 1e-05 0.001 5
## 299:    3180 1e-05 0.001 5
## 300:    3190 1e-05 0.001 5
## 301:    3200 1e-05 0.001 5
## 302:    3210 1e-05 0.001 5
## 303:    3220 1e-05 0.001 5
## 304:    3230 1e-05 0.001 5
## 305:    3240 1e-05 0.001 5
## 306:    3250 1e-05 0.001 5
## 307:    3260 1e-05 0.001 5
## 308:    3270 1e-05 0.001 5
## 309:    3280 1e-05 0.001 5
## 310:    3290 1e-05 0.001 5
## 311:    3300 1e-05 0.001 5
## 312:    3310 1e-05 0.001 5
## 313:    3320 1e-05 0.001 5
## 314:    3330 1e-05 0.001 5
## 315:    3340 1e-05 0.001 5
## 316:    3350 1e-05 0.001 5
## 317:    3360 1e-05 0.001 5
## 318:    3370 1e-05 0.001 5
## 319:    3380 1e-05 0.001 5
## 320:    3390 1e-05 0.001 5
## 321:    3400 1e-05 0.001 5
## 322:    3410 1e-05 0.001 5
## 323:    3420 1e-05 0.001 5
## 324:    3430 1e-05 0.001 5
## 325:    3440 1e-05 0.001 5
## 326:    3450 1e-05 0.001 5
## 327:    3460 1e-05 0.001 5
## 328:    3470 1e-05 0.001 5
## 329:    3480 1e-05 0.001 5
## 330:    3490 1e-05 0.001 5
## 331:    3500 1e-05 0.001 5
## 332:    3510 1e-05 0.001 5
## 333:    3520 1e-05 0.001 5
## 334:    3530 1e-05 0.001 5
## 335:    3540 1e-05 0.001 5
## 336:    3550 1e-05 0.001 5
## 337:    3560 1e-05 0.001 5
## 338:    3570 1e-05 0.001 5
## 339:    3580 1e-05 0.001 5
## 340:    3590 1e-05 0.001 5
## 341:    3600 1e-05 0.001 5
## 342:    3610 1e-05 0.001 5
## 343:    3620 1e-05 0.001 5
## 344:    3630 1e-05 0.001 5
## 345:    3640 1e-05 0.001 5
## 346:    3650 1e-05 0.001 5
## 347:    3660 1e-05 0.001 5
## 348:    3670 1e-05 0.001 5
## 349:    3680 1e-05 0.001 5
## 350:    3690 1e-05 0.001 5
## 351:    3700 1e-05 0.001 5
## 352:    3710 1e-05 0.001 5
## 353:    3720 1e-05 0.001 5
## 354:    3730 1e-05 0.001 5
## 355:    3740 1e-05 0.001 5
## 356:    3750 1e-05 0.001 5
## 357:    3760 1e-05 0.001 5
## 358:    3770 1e-05 0.001 5
## 359:    3780 1e-05 0.001 5
## 360:    3790 1e-05 0.001 5
## 361:    3800 1e-05 0.001 5
## 362:    3810 1e-05 0.001 5
## 363:    3820 1e-05 0.001 5
## 364:    3830 1e-05 0.001 5
## 365:    3840 1e-05 0.001 5
## 366:    3850 1e-05 0.001 5
## 367:    3860 1e-05 0.001 5
## 368:    3870 1e-05 0.001 5
## 369:    3880 1e-05 0.001 5
## 370:    3890 1e-05 0.001 5
## 371:    3900 1e-05 0.001 5
## 372:    3910 1e-05 0.001 5
## 373:    3920 1e-05 0.001 5
## 374:    3930 1e-05 0.001 5
## 375:    3940 1e-05 0.001 5
## 376:    3950 1e-05 0.001 5
## 377:    3960 1e-05 0.001 5
## 378:    3970 1e-05 0.001 5
## 379:    3980 1e-05 0.001 5
## 380:    3990 1e-05 0.001 5
## 381:    4000 1e-05 0.001 5
## 382:    4010 1e-05 0.001 5
## 383:    4020 1e-05 0.001 5
## 384:    4030 1e-05 0.001 5
## 385:    4040 1e-05 0.001 5
## 386:    4050 1e-05 0.001 5
## 387:    4060 1e-05 0.001 5
## 388:    4070 1e-05 0.001 5
## 389:    4080 1e-05 0.001 5
## 390
```

- 11.4 Task: spectral absorbance from spectral transmittance**
- 11.5 Task: spectral transmittance from spectral absorbance**
- 11.6 Task: absorbance from spectral asorbance and spectral irradiance**
- 11.7 Task: reflected spectrum from spectral reflectance and spectral irradiance**
- 11.8 Task: transmitted irradiance**
- 11.9 Task: reflected radiance**
- 11.10 Task: total spectral transmittance from internal spectral transmittance and spectral reflectance**
- 11.11 Task: combined spectral transmittance of two or more filters**
  - Ignoring reflectance
  - Considering reflectance
- 11.12 Task: light scattering media (natural waters, plant and animal tissues)**



## 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.

### 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)
```

### 12.2 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.

### 12.3 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
##      550 nm
## "#00FF00"

w_length2rgb(630) # red
##      630 nm
## "#FF0000"

w_length2rgb(380) # UVA
##      380 nm
## "#000000"

w_length2rgb(750) # far red
##      750 nm
## "#000000"

w_length2rgb(c(550, 630, 380, 750)) # vectorized
##      550 nm      630 nm      380 nm      750 nm
## "#00FF00" "#FF0000" "#000000" "#000000"
```

## 12.4. TASK: CALCULATING AN RGB COLOUR FOR A RANGE OF WAVELENGTHS

### 12.4 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 numbers, 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)

## Warning: Using only extreme wavelength values.

## 400–700 nm
## "#735B57"

w_length_range2rgb(sun.data$w.length)

## Warning: Using only extreme wavelength values.

## 293–800 nm
## "#554340"

w_length_range2rgb(550)

## Warning: Calculating RGB values for monochromatic light.

##      550 nm
## "#00FF00"
```

### 12.5 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.data,
  s_e_irrad2rgb(w.length, s.e.irrad))

## [1] "#544F4B"

with(sun.data,
  s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCMF2.data))

## [1] "#544F4B"

with(sun.data,
  s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCMF10.data))
```

```

## [1] "#59534F"

with(sun.data,
      s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC2.data))

## [1] "#B63C37"

with(sun.data,
      s_e_irrad2rgb(w.length, s.e.irrad, sens=ciexyzCC10.data))

## [1] "#BD3C33"

```

Except for the first example, we specificity the visual sensitivity data to use.

## 12.6 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])

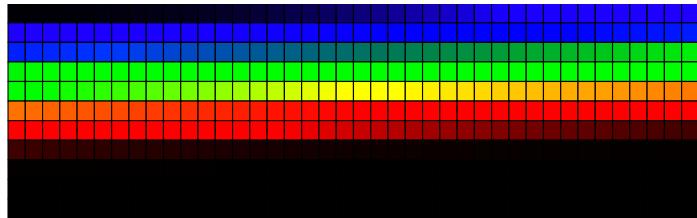
colCount <- 40 # number per row
rowCount <- trunc(length(my.colors) / colCount)

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)])
}

```

RGB colours for 390 to 829 nm





## Photoreceptors

### Abstract

In this chapter we explain how to .

### 13.1 Task:



## Radiation sources

### Abstract

In this chapter we explain how to use the spectral data for light sources.

### 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)
library(photobiologySun)
library(photobiologyLamps)
library(photobiologyLEDs)
library(photobiologyVIS)
library(photobiologyUV)
library(ggplot2)
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(photobiologygg)
```

**14.2 Introduction****14.3 Task: using the data****14.4 Task: extraterrestrial solar radiation spectra****14.5 Task: terrestrial solar radiation spectra****14.6 Task: incandescent lamps****14.7 Task: discharge lamps****14.8 Task: LEDs**

## Filters

### Abstract

In this chapter we explain how to use spectral data for filters and how to convolute it spectral data for light sources.

### 15.1 Packages used in this chapter

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

```
library(photobiology)
library(photobiologyFilters)
library(photobiologySun)
library(photobiologyLamps)
library(photobiologyLEDs)
library(photobiologyVIS)
library(photobiologyUV)
library(ggplot2)
library(ggtern)
library(photobiologygg)
```

### 15.2 Introduction

### 15.3 Task: using the data

### 15.4 Task: spectral transmittance for optical glass filters

### 15.5 Task: spectral transmittance for plastic films

### 15.6 Task: spectral transmittance for plastic sheets



## 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.

### 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(photobiology)
library(photobiologyVIS)
library(photobiologyUV)
library(ggplot2)
library(ggtern)
library(photobiologygg)
library(gridExtra)

## Error: there is no package called 'gridExtra'
```

### 16.2 Introduction to plotting spectra

We show in this chapter examples of how one can plot spectra. All the examples are done with package `ggplot2`, sometimes using in addition other packages. `ggplot2` provides the most recent type 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

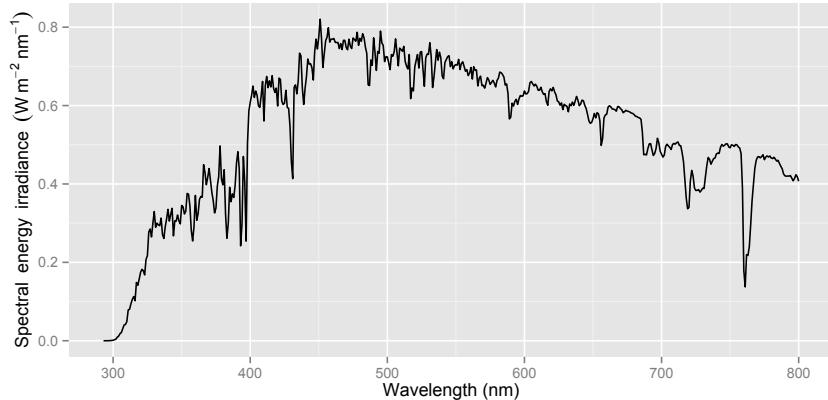
alternatives. Several of the functions used in this chapter are extensions to package `ggplot2`<sup>1</sup>

If you are not familiar with `ggplot2` plotting, please read Appendix C on page 157 before reading the present chapter.

### 16.3 Task: plotting spectra with `ggplot2`

We create a simple line plot, assign it a variable called `fig_sun.e` and then on the next line `print` it. We use `labs` to set nice axis labels.

```
fig_sun.e <-
  ggplot(data=sun.data, aes(x=w.length, y=s.e.irrad)) +
  geom_line() +
  labs(
    y = expression(Spectral~energy~irradiance~~(W~m^{-2}~nm^{-1})) ,
    x = "Wavelength (nm)" )
fig_sun.e
```



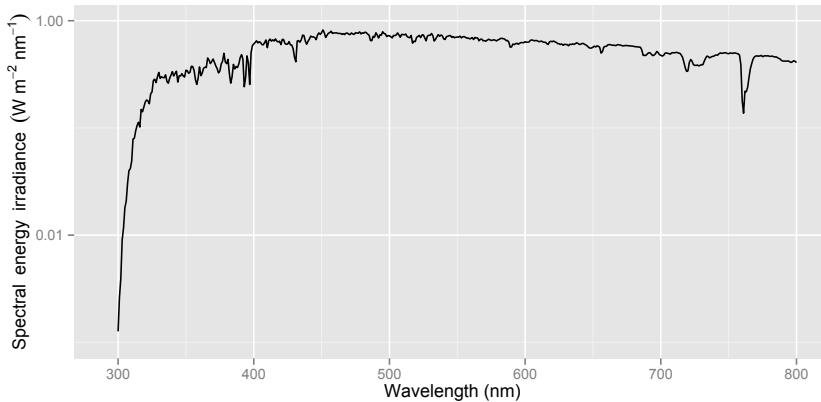
### 16.4 Task: using a log scale

Here without need to recreate the figure, we add a logarithmic scale for the y-axis and print on the fly the result. In this case we override the automatic limits of the scale.

```
fig_sun.e + scale_y_log10(limits=c(1e-3, 1e0))
## Warning: Removed 7 rows containing missing values
(geom_path).
```

---

<sup>1</sup>`ggplot2` is feature-frozen. 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.



## 16.5 Task: compare energy and photon spectral units

We can use function `grid.arrange` to make a single plot from two separate ggplots, and put them side by or on top of each other.

```
theme_stack_opts <-
  list(theme(axis.text.x = element_blank(),
            axis.ticks = element_blank(),
            axis.title.x = element_blank()))
num_one_dec <- function(x, ...)
  format(x, nsmall=1, trim=FALSE, width=4, ...)
fig_sun.q <-
  ggplot(data=sun.data, aes(x=w.length, y=s.q.irrad * 1e6)) +
  geom_line() +
  scale_y_continuous(labels = num_one_dec) +
  labs(y = expression(atop(Spectral~photon~irradiance,
                           (mu*mol~m^-2~s^-1~nm^-1)))) +
  theme_stack_opts
fig_sun.e1 <- fig_sun.e +
  labs(y = expression(atop(Spectral~energy~irradiance,
                           (W~m^-2~nm^-1))),
       x = "Wavelength (nm)")
grid.arrange(fig_sun.q, fig_sun.e1, nrow=2)

## Error:  could not find function "grid.arrange"
```

To make sure that the widths of both plots are the same, we need to make sure that the tick labels in both plots have the same format. For this we define a formatting function `num_one_dec` and then use it at the scale definition. We also add `atop` to the expression to set the spectral irradiance units on a second line in the axis label.

## 16.6 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)<sup>2</sup>. 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.data,
           get_peaks(w.length, s.e.irrad, span=31)))

##      x      y label
## 1 378 0.4970 378
## 2 416 0.6762 416
## 3 451 0.8205 451
## 4 478 0.7870 478
## 5 495 0.7900 495
## 6 531 0.7603 531

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

##      x      y label
## 1 416 0.6762 416
## 2 451 0.8205 451
## 3 478 0.7870 478
## 4 495 0.7900 495
## 5 531 0.7603 531
## 6 582 0.6854 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.data,
           get_peaks(w.length, s.e.irrad, span=21)))

##      x      y label
## 1 354 0.3759 354
## 2 366 0.4492 366
## 3 378 0.4970 378
## 4 416 0.6762 416
## 5 436 0.7337 436
## 6 451 0.8205 451

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

---

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

```
##      x      y label
## 1 451 0.8205   451
## 2 495 0.7900   495
## 3 747 0.5026   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.data,
          get_valleys(w.length, s.e.irrad, span=51)))

##      x      y label
## 1 358 0.2545   358
## 2 393 0.2422   393
## 3 431 0.4137   431
## 4 487 0.6512   487
## 5 517 0.6177   517
## 6 589 0.5659   589

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

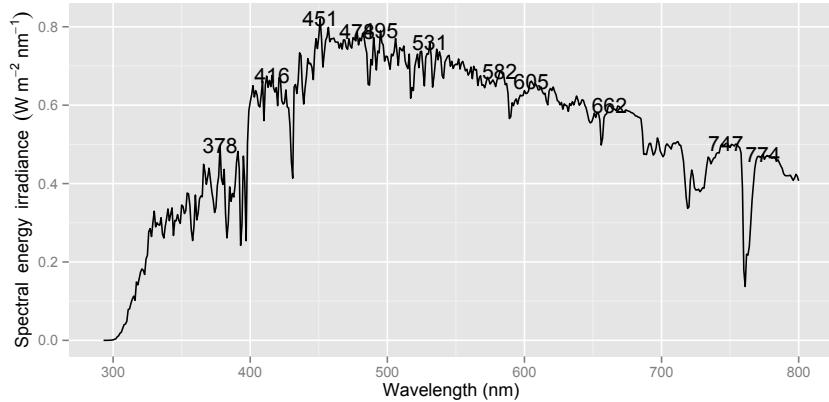
##      x      y label
## 1 431 0.4137   431
## 2 487 0.6512   487
## 3 517 0.6177   517
## 4 589 0.5659   589
## 5 656 0.4983   656
```

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 16.7.

## 16.7 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 16.6. We reuse once more `fig_sun.e` saved in section 16.3.

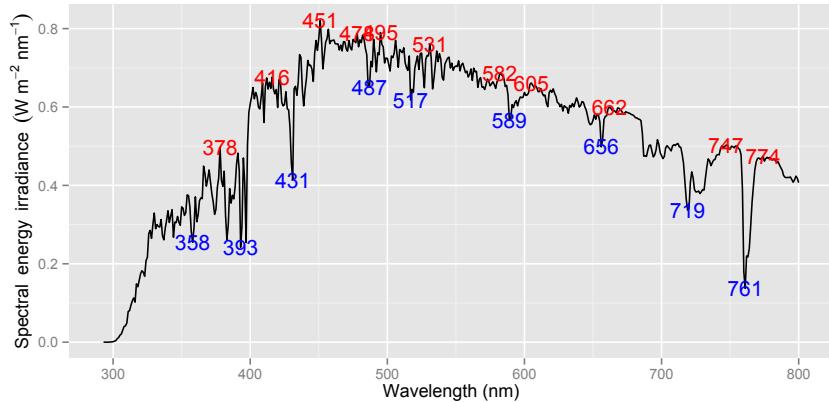
```
fig_sun.e + stat_peaks(span=31)
```



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.

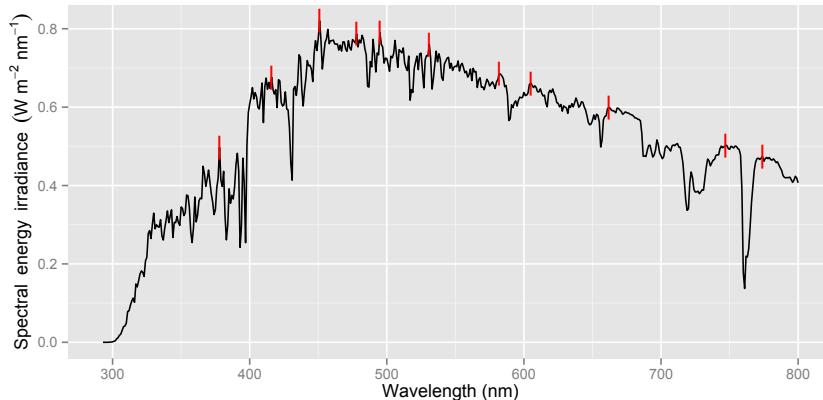
We can change aesthetics, for example the colour:

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

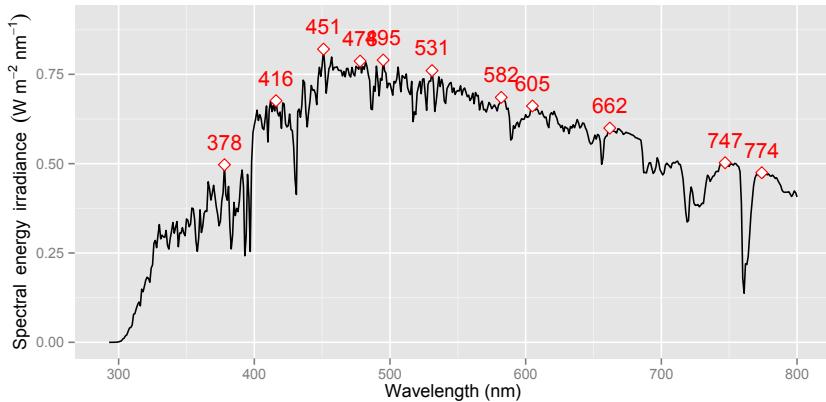


We can add the same `stat` two or more times to a ggplot, in this example, each time with a different `geom`. First we add points to mark the peaks, and afterwards add labels showing the wavelengths at which they are located using `geom "text"`. For the `shape`, or type of symbol, we use one that supports '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<sup>3</sup> In addition we expand the `y`-axis scale so that all labels fall within the plotting area.

```
fig_sun.e +
  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)
```

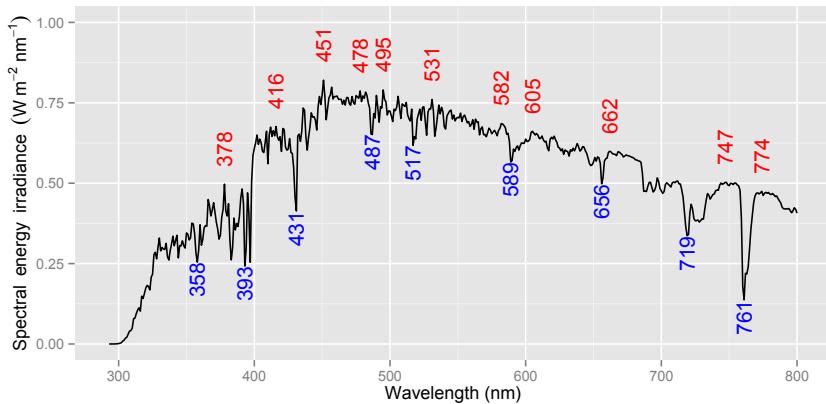
---

<sup>3</sup>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 below 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.e +
  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 14 for an example these stats together with facets.

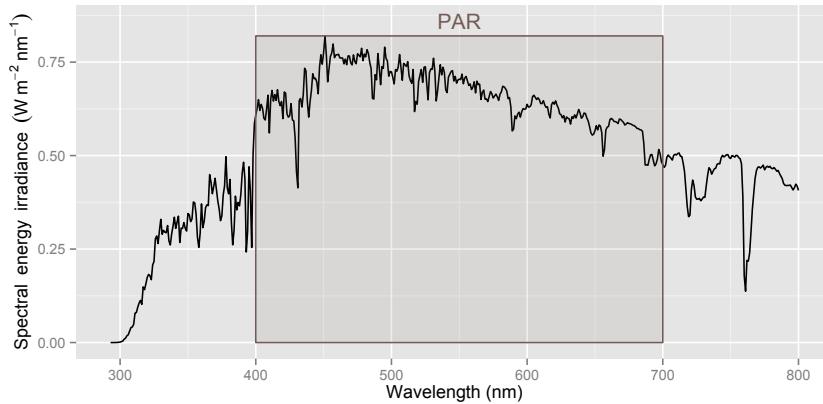
## 16.8 Task: annotating wavebands

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`.

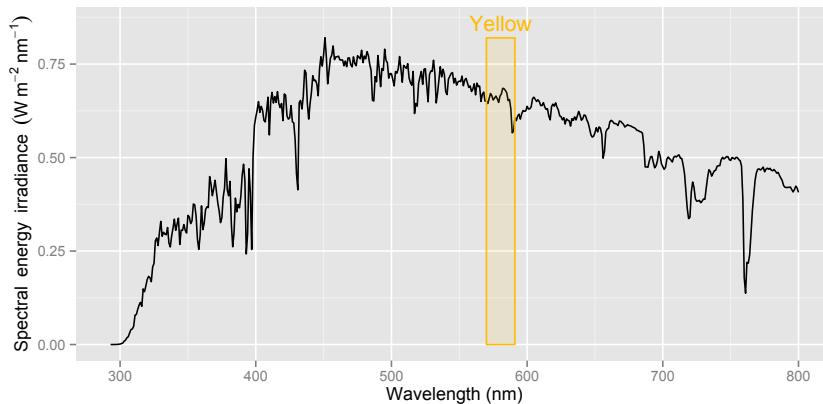
Here is an example for PAR using defaults, and with arguments supplied only for parameters with no defaults. The example does the annotation using two different ‘geoms’, “`rect`” for marking the region, and “`text`” for the labels.

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



This example annotates a narrow waveband.

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

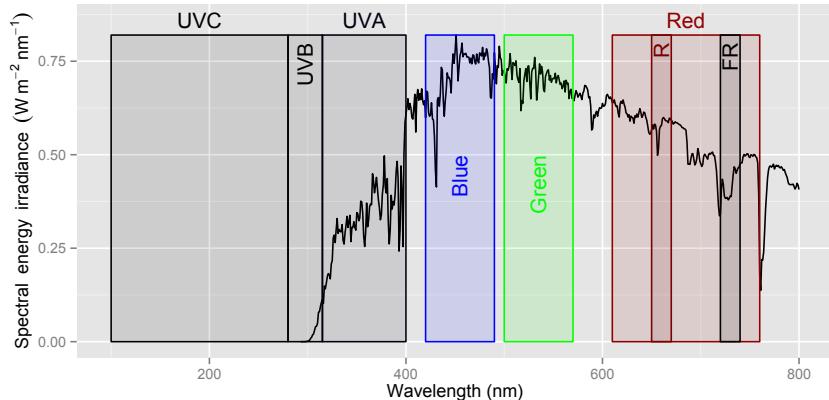


Now an example that is more complex, and demonstrates the flexibility of plots produced with `ggplot2`. We add annotations for eight different wavebands, some of them overlapping. For each one we use two ‘geoms’ and some labels are rotated and justified.

```

figv2 <- fig_sun.e +
  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("Smith"), "rect",
                     ymax=0.82) +
  annotate_waveband(Red("Smith"), "text",
                     y=0.80, angle=90, hjust=1) +
  annotate_waveband(Far_red("Smith"), "rect",
                     ymax=0.82) +
  annotate_waveband(Far_red("Smith"), "text",
                     y=0.80, angle=90, hjust=1)
figv2

```

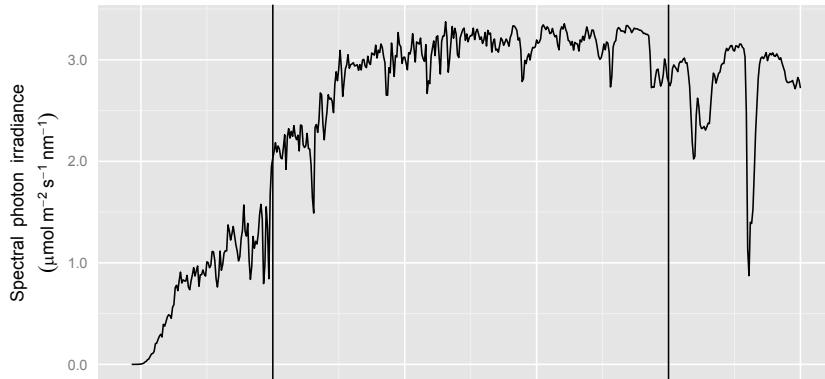


A simple example using `geom_vline`:

```

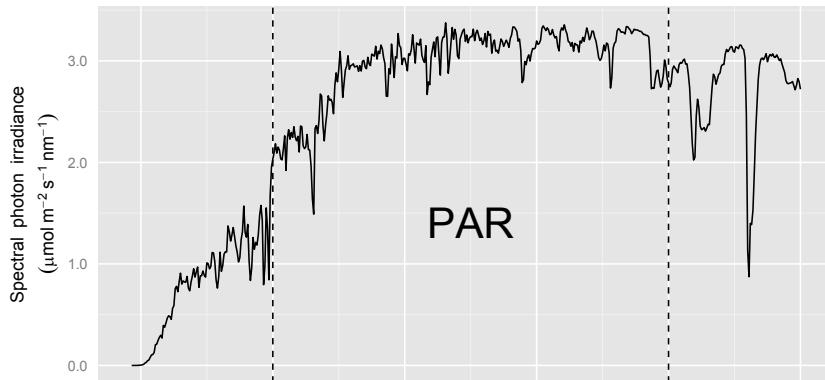
figvl3 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()))
figvl3

```



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

```
figv14 <- fig_sun.q +
  geom_vline(xintercept=range(PAR()), linetype="dashed") +
  annotate_waveband(PAR(), "text", y=1.4, size=10, colour="black")
figv14
```



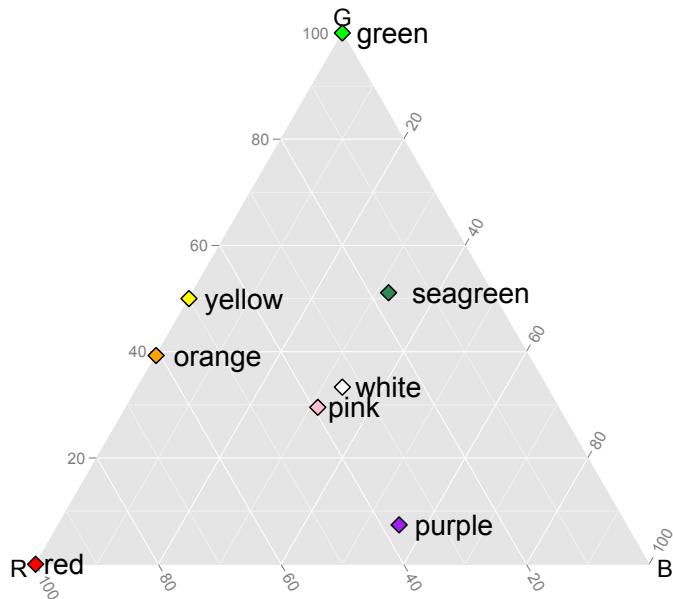
## 16.9 Task: plotting colours in Maxwell's triangle

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 facetting 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_text(hjust=-0.2) +
  labs(x = "R", y="G", z="B") + scale_fill_identity()
maxwell.tern

```



## Calibration

### Abstract

In this chapter we explain how to .

### 17.1 Task:



## Simulation

### Abstract

In this chapter we explain how to .

### 18.1 Task:



## Measurement

### Abstract

In this chapter we explain how to .

### 19.1 Task:



# CHAPTER

# 20

## Optimizing performance

### Abstract

In this chapter we explain how to make your photobiology calculations execute as fast as possible. The code has been profiled and the performance bottlenecks removed in most cases by implementing some functions in C++. Furthermore copying of spectra is minimized by using package `data.table` as the base class of all objects where spectral data is stored. However, it is possible to improve performance even more by changing some defaults and writing efficient user code. This is what is discussed in the present chapter, and should not be of concern unless several thousands of spectra need to be processed.

### 20.1 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(photobiologyVIS)
library(photobiologyUV)
library(microbenchmark)
```

Although not a recommended practice, just to keep the examples shorter, we `attach` a data set for the solar spectrum:

```
attach(sun.data)
## The following objects are masked _by_ .GlobalEnv:
##      s.e.irrad, s.q.irrad
```

## 20.2 Introduction

When developing the current version of photobiology quite a lot of effort was spent in optimizing performance, as in one of our experiments, we need to process several hundreds of thousands of measured spectra. The defaults should provide good performance in most cases, however, some further improvements are achievable, when a series of different calculations are done on the same spectrum, or when a series of spectra measured at exactly the same wavelengths are used for calculating weighted irradiances or exposures.

There is also a lot you can achieve by carefully writing the code in your own scripts. The packages themselves are fairly well optimized for speed. In your own code try to avoid unnecessary copying of big objects. The `r4photobiology` suite makes extensive use of the `data.table` package, using it also in your own code could help. Try to avoid use of explicit loops by replacing them with vectorized operations, and when sequentially building vectors in a loop, preallocate an object big enough before entering the loop.

Being R an interpreted language, there is rather little automatic code optimization taking place, so you may find that even simple things like moving invariant calculations out of loops, and avoiding repeated calculations of the same value by storing the value in a variable can improve performance.

This type of ‘good style’ optimizations have been done throughout the suite’s code, and more specific problem identified by profiling and dealt with case by case. Of course, to achieve maximum overall performance, to should follow the same approach with your own code.

## 20.3 Task: avoiding repeated validation

In the case of doing calculations repeatedly on the same spectrum, a small improvement in performance can be achieved by setting the parameter `check.spectrum=FALSE` for all but the first call to `irradiance()`, or `photon_irradiance()`, or `energy_irradiance()`, or the equivalent functions for ratios. It is also possible to set this parameter to FALSE in all calls, and do the check beforehand by explicitly calling `check_spectrum()`.

## 20.4 Task: caching of multipliers

In the case of calculating weighted irradiances on many spectra having exactly the same wavelength values, then a significant improvement in the performance can be achieved by setting `use.cached.mult=TRUE`, as this reuses the multipliers calculated during successive calls based on the same waveband. However, to achieve this increase in performance, the tests to ensure that the wavelength values have not changed, have to be kept to the minimum. Currently only the length of the wavelength array is checked, and the cached values discarded and recalculated if the length changes. For this reason, this is not the default, and when using caching the user is responsible for making sure that the array of wavelengths has not changed between calls.

## 20.5 Task: benchmarking

You can use the package `microbenchmark` to time the code and find the parts that slow it down. I have used it, and also I have used profiling to optimize the code for speed. The examples below show how choosing different values from the defaults can speed up calculations when the same calculations are done repeatedly on spectra measured at exactly the same wavelengths, something which is usual when analyzing spectra measured with the same instrument. The choice of defaults is based on what is best when processing a moderate number of spectra, say less than a few hundreds, as opposed to many thousands.

```
library(microbenchmark)
```

### Convenience functions

The convenience functions are slightly slower than the generic `irradiance` function.

```
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  irradiance(w.length, s.e.irrad, PAR(), unit.out="photon",
             use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
```

Using the generic reduces the median execution time from 0.11 ms to 0.164 ms, by -49% if using the cache.

### Using cached multipliers

Using the cache when repeatedly applying the same waveband has a large impact on the execution time.

```
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR()),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using an unweighted waveband the cache reduces the median execution time from 0.167 ms to 0.111 ms, by 34%.

When using BSWFs the speed up by use of the cache is more important, and dependent on the complexity of the equation used in the calculation.

```
res1 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, CIE()),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, CIE(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using a weighted waveband, in this example, CIE(), the cache reduces the median execution time from 0.319 ms to 0.123 ms, by 61%.

### Disabling checks

Disabling the checking of the spectrum halves once again the execution time for unweighted wavebands.

```
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
```

When using an unweighted waveband, in this example, PAR(), the disabling the data validation checking reduces the median execution time from 0.112 ms to 0.0796 ms, by 29%.

### Using stored wavebands

Saving a waveband object and reusing it, can give an additional speed up when all other optimizations are also used.

```
myPAR <- PAR()
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, myPAR, use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
```

When using an unweighted waveband, in this example, PAR(), using a saved waveband object reduces the median execution time from 0.0802 ms to 0.0732 ms, by 8.8%.

Saving a waveband object that uses weighting and reusing it, gives an additional speed up when all other optimizations are also used.

```
myCIE <- CIE()
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, CIE(), use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, myCIE, use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
```

When using a weighted waveband, in this example, CIE(), using a saved waveband object reduces the median execution time from 0.0916 ms to 0.0718 ms, by 22%.

### Inserting hinges

Inserting ‘hinges’ to reduce integration errors slows down the computations considerably. If the spectral data is measured with a small wavelength step, the errors are rather small. By default the use of ‘hinges’ is automatically decided based on the average wavelength step in the spectral data. The ‘cost’ of using hinges depends on the waveband definition, as BSWFs with discontinuities in the slope require several hinges, while unweighted one requires at most two, one at each boundary.

```
res1 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, PAR(), use.cache=TRUE,
                     use.hinges=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using an unweighted waveband, in this example, `PAR()`, enabling use of hinges increases the median execution time from 0.112 ms to 0.404 ms, by a factor of 3.6122.

Inserting ‘hinges’ to reduce integration errors slows down the computations a lot. If the spectral data is measured with a small wavelength step, the errors are rather small. By default the use of ‘hinges’ is automatically decided based on the average wavelength step in the spectral data.

```
res1 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, CIE(), use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  energy_irradiance(w.length, s.e.irrad, CIE(), use.cache=TRUE,
                     use.hinges=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using an weighted waveband, in this example, `CIE()`, enabling use of hinges increases the median execution time from 0.123 ms to 0.417 ms, by a factor of 3.3978.

## 20.6 Overall speed-up achievable

### GEN.G

If we consider a slow computation, using a BSWF with a complex equation like `GEN.G`, we can check the best case improvement in throughput that can be —on a given hardware and software system.

```
# slowest
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, GEN.G(),
                     use.cache=FALSE,
                     use.hinges=TRUE,
                     check.spectrum=TRUE),
  times=100L, control=list(warmup = 10L))
```

```
# default
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, GEN.G()),
  times=100L, control=list(warmup = 10L))

# fastest
gen.g <- GEN.G()
res3 <- microbenchmark(
  irradiance(w.length, s.e.irrad, gen.g,
  use.cache=TRUE,
  use.hinges=FALSE,
  check.spectrum=FALSE,
  unit.out="photon"),
  times=100L, control=list(warmup = 10L))
```

When using a weighted waveband, in this example, GEN.G(), enabling all checks and optimizations for precision, and disabling all optimizations for speed yields a median execution time of 0.594 ms, accepting all defaults yields a median execution time 0.294 ms, and disabling all checks, optimizations for precision and enabling all optimizations for speed yields a median execution time of 0.0684, in relation to the slowest one, execution times are 100, 50, and 12%.

Finally we compare the returned values for the irradiance, to see the impact on them of optimizing for speed.

```
# slowest
photon_irradiance(w.length, s.e.irrad, GEN.G(),
  use.cache=FALSE,
  use.hinges=TRUE,
  check.spectrum=TRUE)

## GEN.G.300
## 2.579e-07

# default
photon_irradiance(w.length, s.e.irrad, GEN.G())

## GEN.G.300
## 2.592e-07

# fastest
gen.g <- GEN.G()
irradiance(w.length, s.e.irrad, gen.g,
  use.cache=TRUE,
  use.hinges=FALSE,
  check.spectrum=FALSE,
  unit.out="photon")

## GEN.G.300
## 2.592e-07
```

These results are based on spectral data at 1 nm interval, for more densely measured data the effect of not using hinges becomes even smaller. In contrast, with data measured at wider wavelength steps, the errors will be larger. They also depend on the specific BSWF being used.

## CIE

If we consider a slow computation, using a BSWF with a complex equation like CIE, we can check the best case improvement in throughput that can be —on a given hardware and software system.

```
# slowest
res1 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, CIE(),
    use.cache=FALSE,
    use.hinges=TRUE,
    check.spectrum=TRUE),
    times=100L, control=list(warmup = 10L))

# default
res2 <- microbenchmark(
  photon_irradiance(w.length, s.e.irrad, CIE()),
    times=100L, control=list(warmup = 10L))

# fastest
cie <- CIE()
res3 <- microbenchmark(
  irradiance(w.length, s.e.irrad, cie,
    use.cache=TRUE,
    use.hinges=FALSE,
    check.spectrum=FALSE,
    unit.out="photon"),
    times=100L, control=list(warmup = 10L))
```

When using a weighted waveband, in this example, CIE(), enabling all checks and optimizations for precision, and disabling all optimizations for speed yields a median execution time of 0.635 ms, accepting all defaults yields a median execution time 0.344 ms, and disabling all checks, optimizations for precision and enabling all optimizations for speed yields a median execution time of 0.0692, in relation to the slowest one, execution times are 100, 54, and 11%.

Finally we compare the returned values for the irradiance, to see the impact on them of optimizing for speed.

```
# slowest
photon_irradiance(w.length, s.e.irrad, CIE(),
  use.cache=FALSE,
  use.hinges=TRUE,
  check.spectrum=TRUE)

## CIE98.298
## 2.038e-07

# default
photon_irradiance(w.length, s.e.irrad, CIE())

## CIE98.298
## 2.037e-07

# fastest
CIE <- CIE()
irradiance(w.length, s.e.irrad, CIE,
  use.cache=TRUE,
```

```
use.hinges=FALSE,
check.spectrum=FALSE,
unit.out="photon")

## CIE98.298
## 2.037e-07
```

These results are based on spectral data at 1 nm interval, for more densely measured data the effect of not using hinges becomes even smaller. In contrast, with data measured at wider wavelength steps, the errors will be larger. They also depend on the specific BSWF being used.

### Using `split_irradiance`

Using the cache also helps with `split_irradiance`.

```
res1 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
                          c(400, 500, 600, 700)),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
                          c(400, 500, 600, 700),
                          use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using `split_irradiance`, the cache reduces the median execution time from 0.614 ms to 0.451 ms, by 27%.

Using hinges slows down calculations:

```
res1 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
                          c(400, 500, 600, 700),
                          use.cache=TRUE),
  times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
                          c(400, 500, 600, 700),
                          use.cache=TRUE,
                          use.hinges=TRUE),
  times=100L, control=list(warmup = 10L))
```

When using `split_irradiance`, enabling use of hinges increases the median execution time from 0.443 ms to 0.774 ms, by a factor of 1.7461. There is less overhead than if calculating the same three wavebands separately, as all hinges are inserted in a single operation.

Disabling checking of the spectrum reduces the execution time, but proportionally not as much as for the `irradiance` functions, as the spectrum is checked only once independently of the number of bands into which it is split.

```
res1 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
                          c(400, 500, 600, 700),
                          use.cache=TRUE),
```

```
times=100L, control=list(warmup = 10L))
res2 <- microbenchmark(
  split_photon_irradiance(w.length, s.e.irrad,
    c(400, 500, 600, 700),
    use.cache=TRUE,
    check.spectrum=FALSE),
  times=100L, control=list(warmup = 10L))
```

When using `split_irradiance`, disabling the data validation check reduces the median execution time from 0.449 ms to 0.416 ms, by 7.4%.

As all the execution times are in milliseconds, all the optimizations discussed above are totally irrelevant unless you are planning to repeat similar calculations on thousands of spectra. They apply only to the machine, OS and version of R and packages used when building this typeset output.

## 20.7 Profiling

Profiling is basically fine-grained benchmarking. It provides information about in which part of your code the program spends most time when executing. Once you know this, you can try to just make those critical sections execute faster. Speed-ups can be obtained either by rewriting these parts in a compiled language like C or C++, or by use of a more efficient calculation algorithm. A detailed discussion is outside the scope of this handbook, so only a brief example will be shown here.

```
detach(sun.data)
```



**Part III**

**Appendices**





## R as a powerful calculator

### A.1 Working in the R console

I assume that you are already familiar with RStudio. These examples use only the console window, and results are printed to the console. The values stored in the different variables are also visible in the Environment tab in RStudio.

In the console can type commands at the > prompt. When you end a line by pressing the return key, if the line can be interpreted as an R command, the result will be printed in the console, followed by a new > prompt. If the command is incomplete a + continuation prompt will be shown, and you will be able to type-in the rest of the command. For example if the whole calculation that you would like to do is  $1 + 2 + 4$ , if you enter in the console  $1 + 2 +$  in one line, you will get a continuation prompt where you will be able to type 3. However, if you type  $1 + 2$ , the result will be calculated, and printed.

When working at the command prompt, results are printed by default, but other cases you may need to use the function `print` explicitly. The examples here rely on the automatic printing.

The idea with these examples is that you learn by working out how different commands work based on the results of the example calculations listed. The examples are designed so that they allow the rules, and also a few quirks, to be found by ‘detective work’. This should hopefully lead to better understanding than just studying rules.

### A.2 Examples with numbers

When working with arithmetic expression the normal precedence rules are followed and parentheses can be used to alter this order. In addition parentheses can be nested.

```

1 + 1
## [1] 2

2 * 2
## [1] 4

2 + 10 / 5
## [1] 4
(2 + 10) / 5
## [1] 2.4

10^2 + 1
## [1] 101

sqrt(9)
## [1] 3

pi # whole precision not shown when printing
## [1] 3.142

print(pi, digits=22)
## [1] 3.141592653589793115998

sin(pi) # oops! Read on for explanation.
## [1] 1.225e-16

log(100)
## [1] 4.605

log10(100)
## [1] 2

log2(8)
## [1] 3

exp(1)
## [1] 2.718

```

One can use variables to store values. Variable names and all other names in R are case sensitive. Variables `a` and `A` are two different variables. Variable names can be quite long, but usually it is not a good idea to use very long names. Here I am using very short names, that is usually a very bad idea. However, in cases like these examples where the stored values have no real connection

to the real world and are used just once or twice, these names emphasize the abstract nature.

```
a <- 1
a + 1

## [1] 2

a

## [1] 1

b <- 10
b <- a + b
b

## [1] 11

3e-2 * 2.0

## [1] 0.06
```

There are some syntactically legal statements that are not very frequently used, but you should be aware that they are valid, as they will not trigger error messages, and may surprise you. The important thing is that you write commands consistently. `1 -> a` is valid but almost never used.

```
a <- b <- c <- 0.0
a

## [1] 0

b

## [1] 0

c

## [1] 0

1 -> a
a

## [1] 1

a = 3
a

## [1] 3
```

Numeric variables can contain more than one value. Even single numbers are vectors of length one. We will later see why this is important. As you have seen above the results of calculations were printed preceded with `[1]`. This is the index or position in the vector of the first number (or other value) displayed at the head of the line.

One can use `c` ‘concatenate’ to create a vector of numbers from individual numbers.

```
a <- c(3,1,2)
a
## [1] 3 1 2

b <- c(4,5,0)
b
## [1] 4 5 0

c <- c(a, b)
c
## [1] 3 1 2 4 5 0

d <- c(b, a)
d
## [1] 4 5 0 3 1 2
```

One can also create sequences, or repeat values:

```
a <- -1:5
a
## [1] -1 0 1 2 3 4 5

b <- 5:-1
b
## [1] 5 4 3 2 1 0 -1

c <- seq(from = -1, to = 1, by = 0.1)
c
## [1] -1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2
## [10] -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7
## [19] 0.8 0.9 1.0

d <- rep(-5, 4)
d
## [1] -5 -5 -5 -5
```

Now something that makes R different from most other programming languages: vectorized arithmetic.

```
a + 1 # we add one to vector a defined above
## [1] 0 1 2 3 4 5 6
(a + 1) * 2
## [1] 0 2 4 6 8 10 12
```

```
a + b
## [1] 4 4 4 4 4 4
a - a
## [1] 0 0 0 0 0 0
```

It can be seen in first line above, another peculiarity of R, that frequently called recycling: as vector `a` is of length 6, but the constant 1 is a vector of length 1, this 1 is extended by recycling into a vector of the same length as the longest vector in the statement.

Make sure you understand what calculations are taking place in the chunk above, and also the one below.

```
a <- rep(1, 6)
a

## [1] 1 1 1 1 1 1
a + 1:2
## [1] 2 3 2 3 2 3
a + 1:3
## [1] 2 3 4 2 3 4
a + 1:4
## Warning: longer object length is not a multiple of shorter
##          object length
## [1] 2 3 4 5 2 3
```

A couple on useful things to know: a vector can have length zero. One can remove variables from the workspace with `rm`. One can use `ls` to list all objects in the environment. If you are using RStudio, this same information is visible in the Environment pane.

```
z <- numeric(0)
z

## numeric(0)

ls()

## [1] "a"
## [2] "A2T"
## [3] "b"
## [4] "base"
## [5] "black_body_peak_wl"
## [6] "black_body_spectrum"
## [7] "c"
## [8] "cie"
## [9] "CIE"
```

```

## [10] "colCount"
## [11] "colours"
## [12] "d"
## [13] "day_night.ls"
## [14] "daylengths"
## [15] "daylengths_athens"
## [16] "daylengths_hel"
## [17] "daylengths_ivalo"
## [18] "days"
## [19] "elevations"
## [20] "fig_sun.e"
## [21] "fig_sun.e1"
## [22] "fig_sun.q"
## [23] "figv2"
## [24] "figvl"
## [25] "figvl3"
## [26] "figvl4"
## [27] "filtered_sun.dt"
## [28] "filtered_uncoated_sun.dt"
## [29] "gen.g"
## [30] "geo_code_At"
## [31] "geo_code_BA"
## [32] "geo_code_He"
## [33] "geo_code_Iv"
## [34] "geo_code_Jo"
## [35] "geo_code_Mu"
## [36] "h"
## [37] "hours"
## [38] "i"
## [39] "incl_apdx"
## [40] "incl_chaps"
## [41] "incl_ckbk"
## [42] "j"
## [43] "k.wein"
## [44] "kB"
## [45] "len_days"
## [46] "maxwell.tern"
## [47] "med1"
## [48] "med2"
## [49] "med3"
## [50] "my.colors"
## [51] "my.gg400.dt"
## [52] "my_time"
## [53] "my_version"
## [54] "myCIE"
## [55] "myPAR"
## [56] "num_one_dec"
## [57] "opts_fig_medium"
## [58] "opts_fig_narrow"
## [59] "opts_fig_very_narrow"
## [60] "opts_fig_wide"
## [61] "opts_fig_wide_square"
## [62] "photobio.cache"
## [63] "photobioPhy.cache"
## [64] "photoperiods"
## [65] "Q.RGB"
## [66] "red"
## [67] "remaining"
## [68] "res1"

```

```

## [69] "res2"
## [70] "res3"
## [71] "rgb.values"
## [72] "rowCount"
## [73] "RowSize"
## [74] "s.e.irrad"
## [75] "s.q.irrad"
## [76] "sun_elev_hel"
## [77] "T2A"
## [78] "test.data"
## [79] "theme_stack_opts"
## [80] "toy.wb"
## [81] "twilight"
## [82] "uvb"
## [83] "wb1"
## [84] "wb2"
## [85] "wl"
## [86] "z"

rm(z)
z

## Error: object 'z' not found

ls()

## [1] "a"
## [2] "A2T"
## [3] "b"
## [4] "base"
## [5] "black_body_peak_wl"
## [6] "black_body_spectrum"
## [7] "c"
## [8] "cie"
## [9] "CIE"
## [10] "colCount"
## [11] "colours"
## [12] "d"
## [13] "day_night.ls"
## [14] "daylengths"
## [15] "daylengths_athens"
## [16] "daylengths_hel"
## [17] "daylengths_ivalo"
## [18] "days"
## [19] "elevations"
## [20] "fig_sun.e"
## [21] "fig_sun.e1"
## [22] "fig_sun.q"
## [23] "figv2"
## [24] "figvl"
## [25] "figvl3"
## [26] "figvl4"
## [27] "filtered_sun.dt"
## [28] "filtered_uncoated_sun.dt"
## [29] "gen.g"
## [30] "geo_code_At"
## [31] "geo_code_BA"
## [32] "geo_code_He"
## [33] "geo_code_Iv"
## [34] "geo_code_Jo"

```

```

## [35] "geo_code_Mu"
## [36] "h"
## [37] "hours"
## [38] "i"
## [39] "incl_apdx"
## [40] "incl_chaps"
## [41] "incl_ckbk"
## [42] "j"
## [43] "k.wein"
## [44] "kB"
## [45] "len_days"
## [46] "maxwell.tern"
## [47] "med1"
## [48] "med2"
## [49] "med3"
## [50] "my.colors"
## [51] "my.gg400.dt"
## [52] "my_time"
## [53] "my_version"
## [54] "myCIE"
## [55] "myPAR"
## [56] "num_one_dec"
## [57] "opts_fig_medium"
## [58] "opts_fig_narrow"
## [59] "opts_fig_very_narrow"
## [60] "opts_fig_wide"
## [61] "opts_fig_wide_square"
## [62] "photobio.cache"
## [63] "photobioPhy.cache"
## [64] "photoperiods"
## [65] "Q.RGB"
## [66] "red"
## [67] "remaining"
## [68] "res1"
## [69] "res2"
## [70] "res3"
## [71] "rgb.values"
## [72] "rowCount"
## [73] "RowSize"
## [74] "s.e.irrad"
## [75] "s.q.irrad"
## [76] "sun_elev_hel"
## [77] "T2A"
## [78] "test.data"
## [79] "theme_stack_opts"
## [80] "toy.wb"
## [81] "twilight"
## [82] "uvb"
## [83] "wb1"
## [84] "wb2"
## [85] "wl"

```

There are some special values available for numbers. NA meaning ‘not available’ is used for missing values. Calculations can yield also the following values NaN ‘not a number’, Inf and -Inf for  $\infty$  and  $-\infty$ . As you will see below, calculations yielding these values do **not** trigger errors or warnings, as they are arithmetically valid.

```
a <- NA
a

## [1] NA

-1 / 0

## [1] -Inf

1 / 0

## [1] Inf

Inf / Inf

## [1] NaN

Inf + 4

## [1] Inf
```

One thing to be aware, and which we will discuss again later, is that numbers in computers are almost always stored with finite precision. This means that they not always behave as Real numbers as defined in mathematics. In R the usual numbers are stored as double-precision floats, which means that there are limits to the largest and smallest numbers that can be represented (approx.  $-1 \cdot 10^{308}$  and  $1 \cdot 10^{308}$ ), and the number of significant digits that can be stored (usually described as  $\epsilon$  (epsilon, abbreviated `eps`, defined as the smallest number for which  $1 + \epsilon = 1$ )). This can be sometimes important, and can generate unexpected results in some cases, especially when testing for equality. In the example below, the result of the subtraction is still exactly 1.

```
1 - 1e-20

## [1] 1
```

### A.3 Examples with logical values

What in maths are usually called Boolean values, are called `logical` values in R. They can have only two values `TRUE` and `FALSE`, in addition to `NA`. They are vectors. There are also logical operators that allow boolean algebra (and some support for set operations that we will not describe here).

```
a <- TRUE
b <- FALSE
a

## [1] TRUE

!a # negation

## [1] FALSE
```

```
a && b # logical AND
## [1] FALSE
a || b # logical OR
## [1] TRUE
```

Again vectorization is possible. I present this here, and will come back again to this, because this is one of the most troublesome aspects of the R language. The two types of ‘equivalent’ logical operators behave very differently, but use very similar syntax!

```
a <- c(TRUE, FALSE)
b <- c(TRUE, TRUE)
a

## [1] TRUE FALSE

b

## [1] TRUE TRUE

a & b # vectorized AND
## [1] TRUE FALSE

a | b # vectorized OR
## [1] TRUE TRUE

a && b # not vectorized
## [1] TRUE

a || b # not vectorized
## [1] TRUE

any(a)
## [1] TRUE

all(a)
## [1] FALSE

any(a & b)
## [1] TRUE

all(a & b)
## [1] FALSE
```

Another important thing to know about logical operators is that they ‘short-cut’ evaluation. If the result is known from the first part of the statement, the

rest of the statement is not evaluated. Try to understand what happens when you enter the following commands.

```
TRUE & FALSE & NA
## [1] FALSE

TRUE && FALSE && NA
## [1] FALSE

TRUE && TRUE && NA
## [1] NA

a & b & c(NA, NA)
## [1] NA FALSE
```

## A.4 Comparison operators

Comparison operators yield as a result logical values.

```
1.2 > 1.0
## [1] TRUE

1.2 >= 1.0
## [1] TRUE

1.2 == 1.0 # be aware that here we use two = symbols
## [1] FALSE

1.2 != 1.0
## [1] TRUE

1.2 <= 1.0
## [1] FALSE

1.2 < 1.0
## [1] FALSE

a <- 20
a < 100 && a > 10
## [1] TRUE
```

Again these operators can be used on vectors of any length, the result is a logical vector.

```

a <- 1:10
a > 5

## [1] FALSE FALSE FALSE FALSE FALSE TRUE TRUE
## [8] TRUE TRUE TRUE

a < 5

## [1] TRUE TRUE TRUE TRUE FALSE FALSE FALSE
## [8] FALSE FALSE FALSE

a == 5

## [1] FALSE FALSE FALSE FALSE TRUE FALSE FALSE
## [8] FALSE FALSE FALSE

all(a > 5)

## [1] FALSE

any(a > 5)

## [1] TRUE

b <- a > 5
b

## [1] FALSE FALSE FALSE FALSE FALSE TRUE TRUE
## [8] TRUE TRUE TRUE

any(b)

## [1] TRUE

all(b)

## [1] FALSE

```

Be once more aware of ‘short-cut evaluation’. If the result would not be affected by the missing value then the result is returned. If the presence of the NA makes the end result unknown, then NA is returned.

```

c <- c(a, NA)
c > 5

## [1] FALSE FALSE FALSE FALSE FALSE FALSE TRUE TRUE
## [8] TRUE TRUE TRUE NA

all(c > 5)

## [1] FALSE

any(c > 5)

## [1] TRUE

all(c < 20)

```

```

## [1] NA
any(c > 20)
## [1] NA
is.na(a)
## [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [8] FALSE FALSE FALSE
is.na(c)
## [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [8] FALSE FALSE FALSE TRUE
any(is.na(c))
## [1] TRUE
all(is.na(c))
## [1] FALSE

```

This behaviour can be changed by using the optional argument `na.rm` which removes NA values **before** the function is applied. (Many functions in R have this optional parameter.)

```

all(c < 20)
## [1] NA
any(c > 20)
## [1] NA
all(c < 20, na.rm=TRUE)
## [1] TRUE
any(c > 20, na.rm=TRUE)
## [1] FALSE

```

You may skip this on first read, see page 113.

```

1e20 == 1 + 1e20
## [1] TRUE
1 == 1 + 1e-20
## [1] TRUE
0 == 1e-20
## [1] FALSE

```

In many situations, when writing programs one should avoid testing for equality of floating point numbers ('floats'). Here we show how to handle gracefully rounding errors.

```
a == 0.0 # may not always work
## [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [8] FALSE FALSE FALSE

abs(a) < 1e-15 # is safer
## [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [8] FALSE FALSE FALSE

sin(pi) == 0.0 # angle in radians, not degrees!
## [1] FALSE

sin(2 * pi) == 0.0
## [1] FALSE

abs(sin(pi)) < 1e-15
## [1] TRUE

abs(sin(2 * pi)) < 1e-15
## [1] TRUE

sin(pi)
## [1] 1.225e-16

sin(2 * pi)
## [1] -2.449e-16

.Machine$double.eps # see help for .Machine for explanation
## [1] 2.22e-16

.Machine$double.neg.eps
## [1] 1.11e-16
```

## A.5 Character values

Character variables can be used to store any character. Character constants are written by enclosing characters in quotes. There are three types of quotes in the ASCII character set, double quotes ", single quotes ', and back ticks `'. The first two types of quotes can be used for delimiting characters.

```
a <- "A"
b <- letters[2]
```

```
c <- letters[1]
a

## [1] "A"

b

## [1] "b"

c

## [1] "a"

d <- c(a, b, c)
d

## [1] "A" "b" "a"

e <- c(a, b, "c")
e

## [1] "A" "b" "c"

h <- "1"
h + 2

## Error: non-numeric argument to binary operator
```

Vectors of characters are not the same as character strings.

```
f <- c("1", "2", "3")
g <- "123"
f == g

## [1] FALSE FALSE FALSE

f

## [1] "1" "2" "3"

g

## [1] "123"
```

Skip this on first read, but look at this again later because it can be useful in some cases.

One can use the ‘other’ type of quotes as delimiter when one want to include quotes in a string. Pretty-printing is changing what I typed into how the string is stored in R: I typed `b <- 'He said "hello" when he came in'`, try it.

```
a <- "He said 'hello' when he came in"
a

## [1] "He said 'hello' when he came in"

b <- 'He said "hello" when he came in'
b
```

```
## [1] "He said \"hello\" when he came in"
```

The outer quotes are not part of the string, they are ‘delimiters’ used to mark the boundaries. As you can see when b is printed special characters can be represented using ‘escape sequences’. There are several of them, and here we will show just a few.

```
c <- "abc\n\tdef\txyz"
c

## [1] "abc\n\tdef\txyz"
```

Above, you will not see any effect of these escapes: `\n` represents ‘new line’ and `\t` means ‘tab’ (tabulator). These work only in some contexts, but they can be useful for example when one wants to split an axis-label in a plot into two lines.

## A.6 Type conversions

The least intuitive ones are those related to logical values. All others are as one would expect.

```
as.character(1)

## [1] "1"

as.character(3.0e10)

## [1] "3e+10"

as.numeric("1")

## [1] 1

as.numeric("5E+5")

## [1] 5e+05

as.numeric("A")

## Warning:  NAs introduced by coercion

## [1] NA

as.numeric(TRUE)

## [1] 1

as.numeric(FALSE)

## [1] 0

TRUE + TRUE

## [1] 2

TRUE + FALSE

## [1] 1
```

```
TRUE * 2
## [1] 2

FALSE * 2
## [1] 0

as.logical("T")
## [1] TRUE

as.logical("t")
## [1] NA

as.logical("TRUE")
## [1] TRUE

as.logical("true")
## [1] TRUE

as.logical(100)
## [1] TRUE

as.logical(0)
## [1] FALSE

as.logical(-1)
## [1] TRUE
```

```
f <- c("1", "2", "3")
g <- "123"
as.numeric(f)

## [1] 1 2 3

as.numeric(g)

## [1] 123
```

Some tricks useful when dealing with results. Be aware that the printing is being done by default, these functions return numerical values.

```
round(0.0124567, 3)
## [1] 0.012

round(0.0124567, 1)
## [1] 0
```

```

round(0.0124567, 5)
## [1] 0.01246

signif(0.0124567, 3)
## [1] 0.0125

round(1789.1234, 3)
## [1] 1789

signif(1789.1234, 3)
## [1] 1790

a <- 0.12345
b <- round(a, 2)
a == b

## [1] FALSE

a - b

## [1] 0.00345

b

## [1] 0.12

```

## A.7 Vectors

You already know how to create a vector. Now we are going to see how to get individual numbers out of a vector. They are accessed using an index. The index indicates the position in the vector, starting from one, following the usual mathematical tradition. What in maths would be  $x_i$  for a vector  $x$ , in R is represented as `x[i]`. (Some other computer languages use indexes that start at zero.)

```

a <- letters[1:10]
a

## [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[ ]
## [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[numeric(0)] # a bit tricky

## character(0)

a[NA]

## [1] NA NA

```

```
a[c(1, NA)]
## [1] "a" NA

a[2]
## [1] "b"

a[c(3,2)]
## [1] "c" "b"

a[10:1]
## [1] "j" "i" "h" "g" "f" "e" "d" "c" "b" "a"
a[c(3,3,3,3)]
## [1] "c" "c" "c" "c"

a[c(10:1, 1:10)]
## [1] "j" "i" "h" "g" "f" "e" "d" "c" "b" "a" "a"
## [12] "b" "c" "d" "e" "f" "g" "h" "i" "j"
```

Another way of indexing, which is very handy, but not available in most other computer languages, is indexing with a vector of logical values. In practice, the vector of logical values used for ‘indexing’ is in most cases of the same length as the vector from which elements are going to be selected. However, this is not a requirement, and if one vector is short it is ‘recycled’ as discussed above in relation to operators.

```
a[TRUE]
## [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[FALSE]
## character(0)

a[c(TRUE, FALSE)]
## [1] "a" "c" "e" "g" "i"

a[c(FALSE, TRUE)]
## [1] "b" "d" "f" "h" "j"

a > "c"
## [1] FALSE FALSE FALSE TRUE  TRUE  TRUE  TRUE
## [8] TRUE  TRUE  TRUE

a[a > "c"]
## [1] "d" "e" "f" "g" "h" "i" "j"
```

```

selector <- a > "c"
a[selector]

## [1] "d" "e" "f" "g" "h" "i" "j"

which(a > "c")

## [1] 4 5 6 7 8 9 10

indexes <- which(a > "c")
a[indexes]

## [1] "d" "e" "f" "g" "h" "i" "j"

b <- 1:10
b[selector]

## [1] 4 5 6 7 8 9 10

b[indexes]

## [1] 4 5 6 7 8 9 10

```

## A.8 Simple built-in statistical functions

Being R's main focus in statistics, it provides functions for both simple and complex calculations, going from means and variances to fitting very complex models. we will start with the simple ones.

```

x <- 1:20
mean(x)

## [1] 10.5

var(x)

## [1] 35

median(x)

## [1] 10.5

mad(x)

## [1] 7.413

sd(x)

## [1] 5.916

range(x)

## [1] 1 20

max(x)

```

```
## [1] 20  
  
min(x)  
## [1] 1  
  
length(x)  
## [1] 20
```

## A.9 Functions and execution flow control

Although functions can be defined and used at the command prompt, we will discuss them when looking at scripts. We will do the same in the case of flow-control statements (e.g. repetition and conditional execution).





## R Scripts and Programming

### B.1 What is script?

We call *script* to a text file that contains the same commands that you would type at the console prompt. A true script is not for example an MS-Word file where you have pasted or typed some R commands. A script file has the following characteristics.

- The script is a text file (ASCII or some other encoding e.g. UTF-8 that R uses in your set-up).
- The file contains valid R statements (including comments) and nothing else.
- Comments start at a # and end at the end of the line. (True end-of line as coded in file, the editor may wrap it or not at the edge of the screen).
- The R statements are in the file in the order that they must be executed.
- R scripts have file names ending in .r

It is good practice to write scripts so that they will run in a new R session, which means that the script should include library commands to load all the required packages.

### B.2 How do we use a script?

A script can be sourced.

If we have a text file called `my.first.script.r`

```
# this is my first R script  
print(3+4)
```

And then source this file:

```
source("my.first.script.r")
## [1] 7
```

The results of executing the statements contained in the file will appear in the console. The commands themselves are not shown (the sourced file is not echoed) and the results will not be printed unless you include an explicit `print` command. This also applies in many cases also to plots. A fig created with `ggplot` needs to be printed if we want to see it when the script is run.

From within RStudio, if you have an R script open in the editor, there will a “source” drop box (= DropBox) visible from where you can choose “source” as described above, or “source with echo” for the currently open file.

When a script is sourced, the output can be saved to a text file instead of being shown in the console. It is also easy to call R with the script file as argument directly at the command prompt of the operating system.

```
RScript my.first.script.r
```

You can open a ‘shell’ from the Tools menu in RStudio, to run this command. The output will be printed to the shell console. If you would like to save the output to a file, use redirection.

```
RScript my.first.script.r > my.output.txt
```

Sourcing is very useful when the script is ready, however, while developing a script, or sometimes when testing things, one usually wants to run (= execute) one or a few statements at a time. This can be done using the “run” button after either locating the cursor in the line to be executed, or selecting the text that one would like to run (the selected text can be part of a line, a whole line, or a group of lines, as long as it is syntactically valid).

### B.3 How to write a script?

The approach used, or mix of approaches will depend on your preferences, and on how confident you are that the statements will work as expected.

**If one is very familiar with similar problems** One would just create a new text file and write the whole thing in the editor, and then test it. This is rather unusual.

**If one is moderately familiar with the problem** One would write the script as above, but testing it, part by part as one is writing it. This is usually what I do.

**If ones mostly playing around** Then if one is using RStudio, one type statements at the console prompt. As you should know by now, everything you run at the console is saved to the “History”. In RStudio the History is displayed in its own pane, and in this pane one can select any previous

statement and by pressing a single having copy and pasted to either the console prompt, or the cursor position in the file visible in the editor. In this way one can build a script by copying and pasting from the history to your script file the bits that have worked as you wanted.

## B.4 The need to be understandable to people

When you write a script, it is either because you want to document what you have done or you want re-use it at a later time. In either case, the script itself although still meaningful for the computer could become very obscure to you, and even more to someone seeing it for the first time.

How does one achieve an understandable script or program?

- Avoid the unusual. People using a certain programming language tend to use some implicit or explicit rules of style. As a minimum try to be consistent with yourself.
- Use meaningful names for variables, and any other object. What is meaningful depends on the context. Depending on common use a single letter may be more meaningful than a long word. However self explaining names are better: e.g. using `n.rows` and `n.cols` is much clearer than using `n1` and `n2` when dealing with a matrix of data. Probably `number.of.rows` and `number.of.columns` would just increase the length of the lines in the script, and one would spend more time typing without getting much in return.
- How to make the words visible in names: traditionally in R one would use dots to separate the words and use only lower case. Some years ago, it became possible to use underscores. The use of underscores is quite common nowadays because in some contexts is “safer” as in special situations a dot may have a special meaning. What we call “camel case” is very rarely used in R programming but is common in other languages like Pascal. An example of camel case is `NumCol.s`. In some cases it can become a bit confusing as in `UVMean` or `UvMean`.

## B.5 Exercises

By now you should be familiar enough with R to be able to write your own script.

1. Create a new R script (in RStudio, from ‘File’ menu, “+” button, or by typing “Ctrl + Shift + N”).
2. Save the file as “`my.second.script.r`”.
3. Use the editor pane in RStudio to type some R commands and comments.
4. **Run** individual commands.
5. **Source** the whole file.

## B.6 Functions

When writing scripts, or any program, one should avoid repeating code (groups of statements). The reasons for this are: 1) if the code needs to be changed, you have to make changes in more than one place in the file, or in more than one file. Sooner or later, some copies will remain unchanged by mistake. 2) it makes the script file longer, and this makes debugging, commenting, etc. more tedious, and error prone.

How do we avoid repeating bits of code? We write a function containing the statements that we would need to repeat, and then `call` the function in their place.

Functions are defined by means of `function`, and saved like any other object in R by assignment a variable. `x` is a parameter, the name used within the function for an object that will be supplied as “argument” when the function is called. One can think of parameter names as place-holders.

```
my.prod <- function(x, y){x * y}
my.prod(4, 3)

## [1] 12
```

First some basic knowledge. In R, arguments are passed by copy. This is something very important to remember. Whatever you do within a function to the passed argument, its value outside the function will remain unchanged.

```
my.change <- function(x){x <- NA}
a <- 1
my.change(a)
a

## [1] 1
```

Any result that needs to be made available outside the function must be returned by the function. If the function `return` is not explicitly used, the value returned by the last statement within the body of the function will be returned.

```
print.x.1 <- function(x){print(x)}
print.x.1("test")

## [1] "test"

print.x.2 <- function(x){print(x); return(x)}
print.x.2("test")

## [1] "test"
## [1] "test"

print.x.3 <- function(x){return(x); print(x)}
print.x.3("test")

## [1] "test"

print.x.4 <- function(x){return(); print(x)}
print.x.4("test")

## NULL
```

We can assign to a variable defined outside a function with operator `<-` – but the usual recommendation is to avoid its use. This type of effects of calling a function are frequently called ‘side-effects’.

Now we will define a useful function: a function for calculating the standard error of the mean from a numeric vector.

```
SEM <- function(x){sqrt(var(x)/length(x))}
a <- c(1, 2, 3, -5)
a.na <- c(a, NA)
SEM(x=a)

## [1] 1.797

SEM(a)

## [1] 1.797

SEM(a.na)

## [1] NA
```

For example in `SEM(a)` we are calling function `SEM` with `a` as argument.

The function we defined above may sometimes give a wrong answer because NAs will be counted by `length`, so we need to remove NAs before calling `length`.

```
SEM <- function(x) sqrt(var(x, na.rm=TRUE)/length(na.omit(x)))
a <- c(1, 2, 3, -5)
a.na <- c(a, NA)
SEM(x=a)

## [1] 1.797

SEM(a)

## [1] 1.797

SEM(a.na)

## [1] 1.797
```

R does not have a function for standard error, so the function above would be generally useful. If we would like to make this function both safe, and consistent with other R functions, one could define it as follows, allowing the user to provide a second argument which is passed as an argument to `var`:

```
SEM <- function(x, na.rm=FALSE){sqrt(var(x, na.rm=na.rm)/length(na.omit(x)))}
SEM(a)

## [1] 1.797

SEM(a.na)

## [1] NA

SEM(a.na, TRUE)
```

```

## [1] 1.797
SEM(x=a.na, na.rm=TRUE)
## [1] 1.797
SEM(TRUE, a.na)
## Warning: the condition has length > 1 and only the first
## element will be used
## [1] NA
SEM(na.rm=TRUE, x=a.na)
## [1] 1.797

```

In this example you can see that functions can have more than one parameter, and that parameters can have default values to be used if no argument is supplied. In addition if the name of the parameter is indicated, then arguments can be supplied in any order, but if parameter names are not supplied, then arguments are assigned to parameters based on their position. Once one parameter name is given, all later arguments need also to be explicitly matched to parameters. Obviously if given by position, then arguments should be supplied explicitly for all parameters at ‘intermediate’ positions.

## B.7 R built-in functions

### Plotting

The built-in generic function `plot` can be used to plot data. It is a generic function, that has suitable methods for different kinds of objects.

Before we can plot anything, we need some data.

```

data(cars)
names(cars)

## [1] "speed" "dist"

head(cars)

##      speed dist
## 1      4     2
## 2      4    10
## 3      7     4
## 4      7    22
## 5      8    16
## 6      9    10

tail(cars)

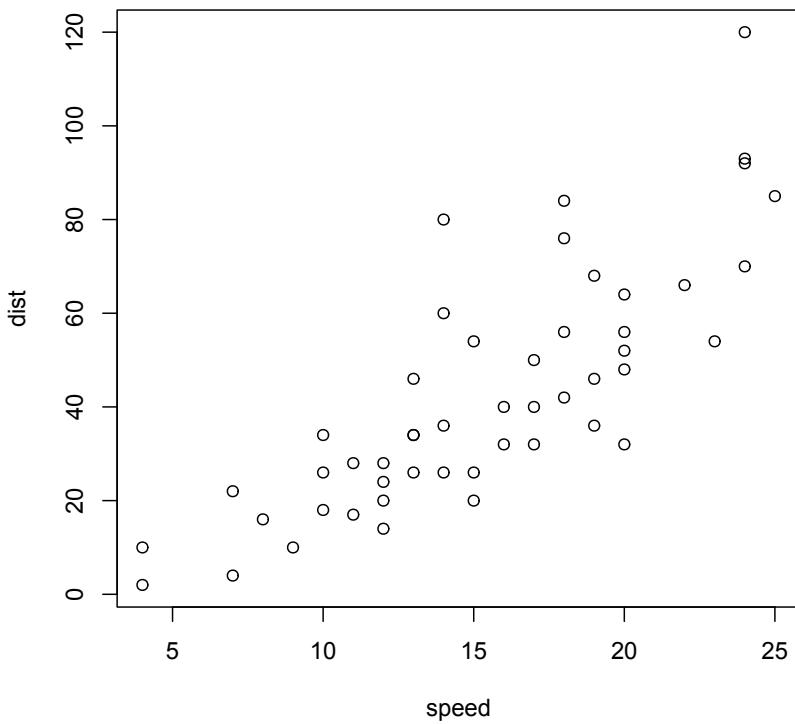
##      speed dist
## 45     23    54
## 46     24    70
## 47     24    92

```

```
## 48     24    93
## 49     24   120
## 50     25    85
```

`cars` is an example data set that is included in R. It is stored as a data frame. Data frames are used for storing data, they consist in columns of equal length. The different columns can be different types (e.g. numeric and character). With `data` we load it; with `names` we obtain the names of the variables or columns. With `head` with can see the top several lines, and with `tail` the lines at the end.

```
plot(dist ~ speed, data=cars)
```



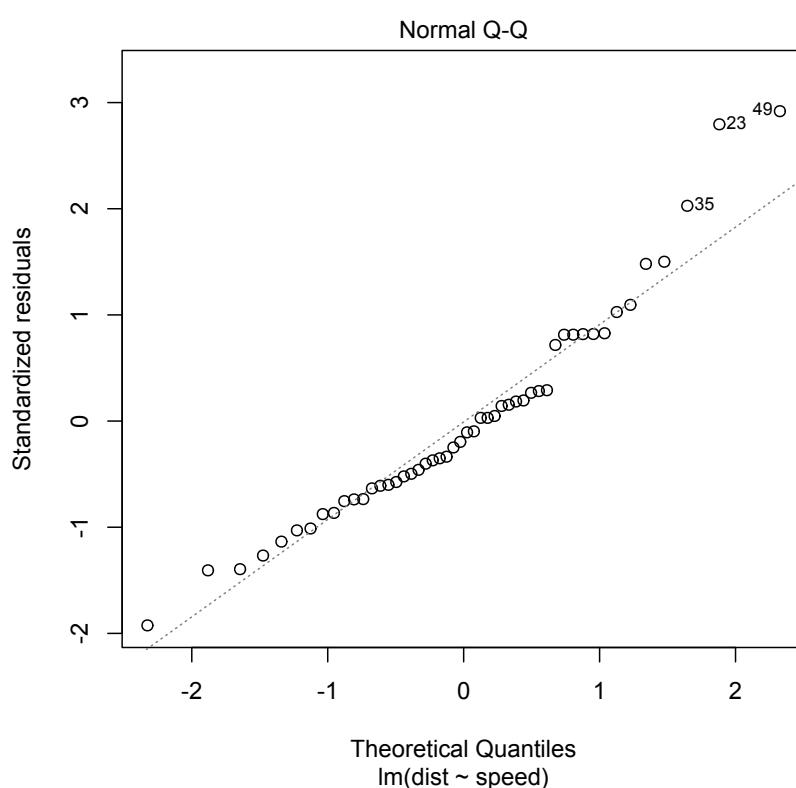
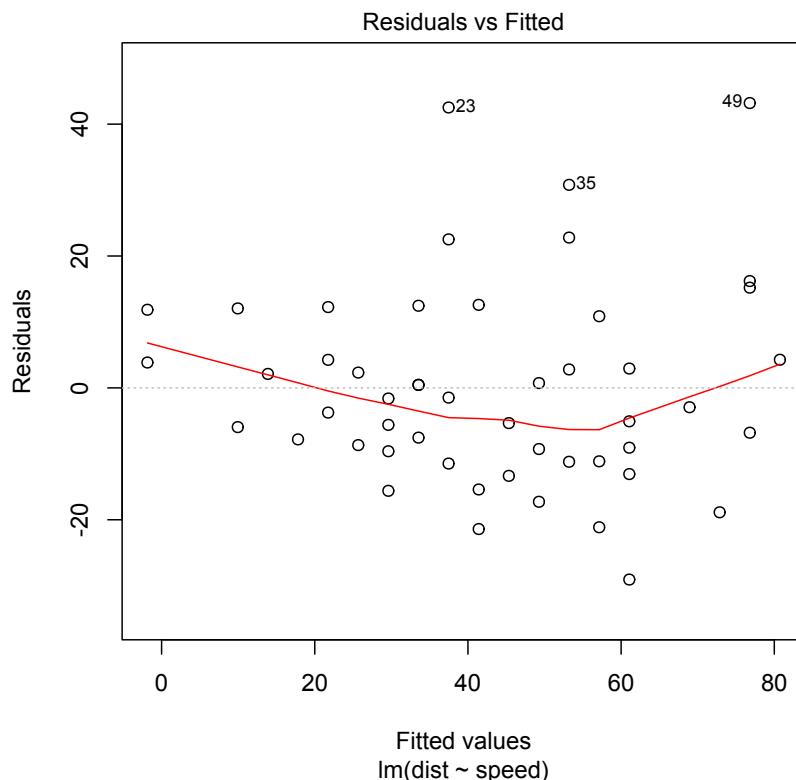
## Fitting linear models

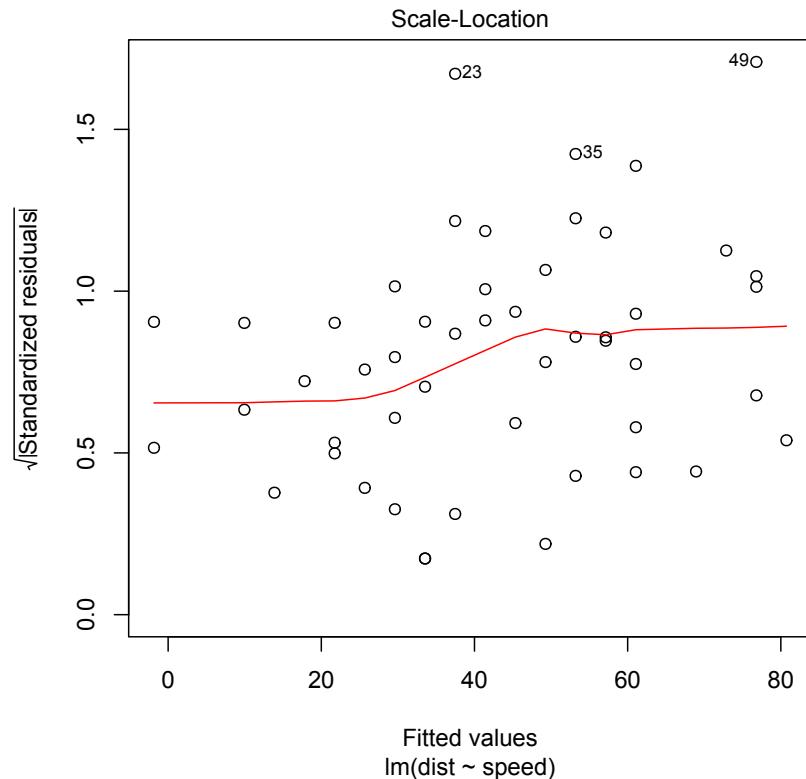
### Regression

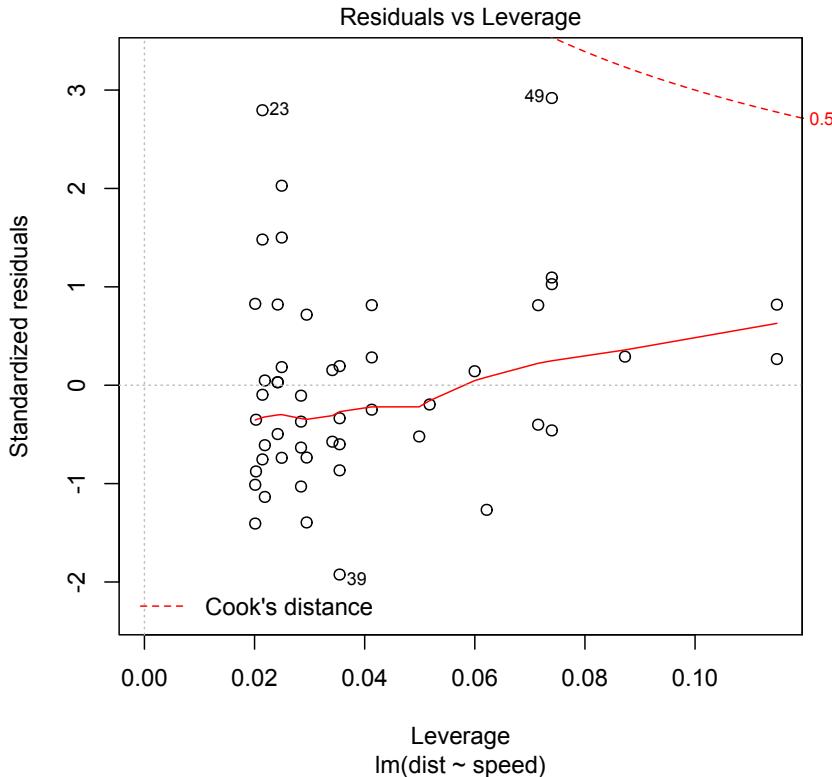
The R function `lm` is used next to fit a linear regression.

```
fm1 <- lm(dist ~ speed, data=cars) # we fit a model, and then save the result
plot(fm1) # we produce diagnosis plots
summary(fm1) # we inspect the results from the fit
##
```

```
## Call:  
## lm(formula = dist ~ speed, data = cars)  
##  
## Residuals:  
##    Min     1Q Median     3Q    Max  
## -29.07  -9.53  -2.27   9.21  43.20  
##  
## Coefficients:  
##              Estimate Std. Error t value Pr(>|t|)  
## (Intercept) -17.579     6.758  -2.60   0.012  
## speed         3.932     0.416   9.46  1.5e-12  
##  
## (Intercept) *  
## speed      ***  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1  
##  
## Residual standard error: 15.4 on 48 degrees of freedom  
## Multiple R-squared:  0.651, Adjusted R-squared:  0.644  
## F-statistic: 89.6 on 1 and 48 DF,  p-value: 1.49e-12  
  
anova(fm1) # we calculate an ANOVA  
  
## Analysis of Variance Table  
##  
## Response: dist  
##             Df Sum Sq Mean Sq F value Pr(>F)  
## speed       1  21185   21185    89.6 1.5e-12 ***  
## Residuals  48  11354    237  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```







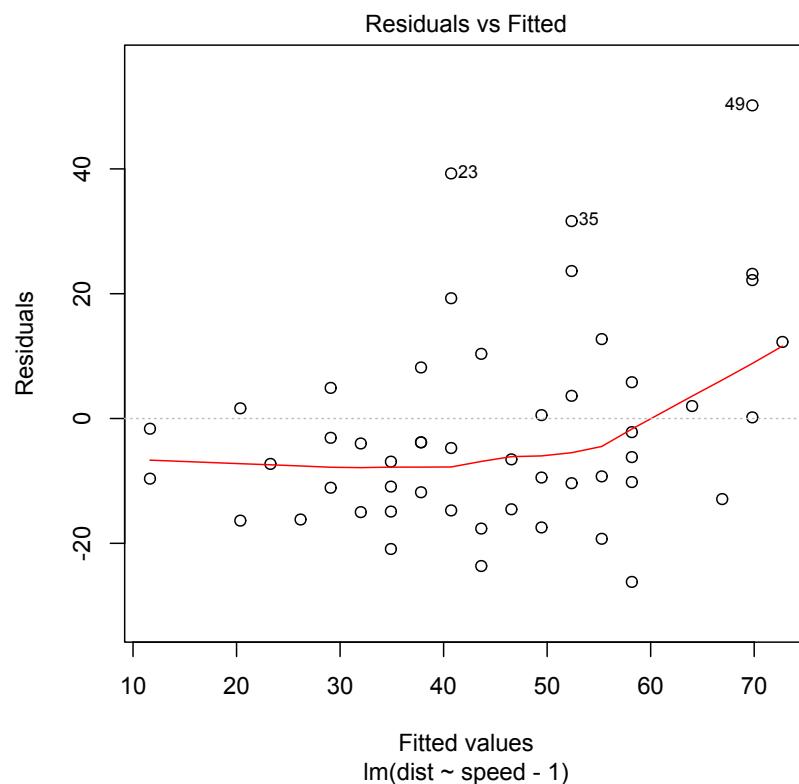
Let's look at each step separately: `dist ~ speed` is the specification of the model to be fitted. The intercept is always implicitly included. To 'remove' this implicit intercept from the earlier model we can use `dist ~ speed - 1`.

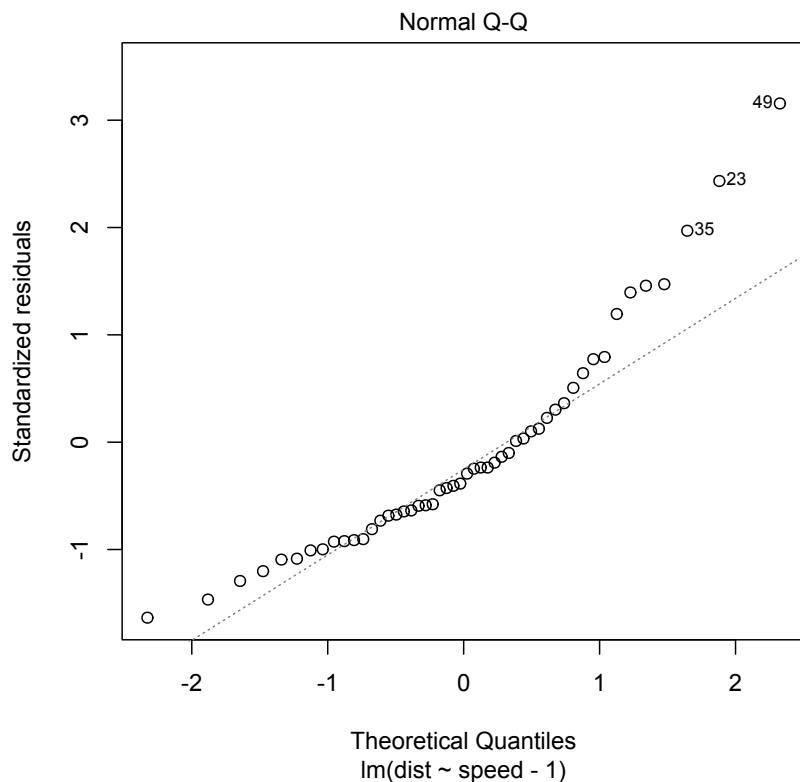
```
fm2 <- lm(dist ~ speed - 1, data=cars) # we fit a model, and then save the result
plot(fm2) # we produce diagnosis plots
summary(fm2) # we inspect the results from the fit

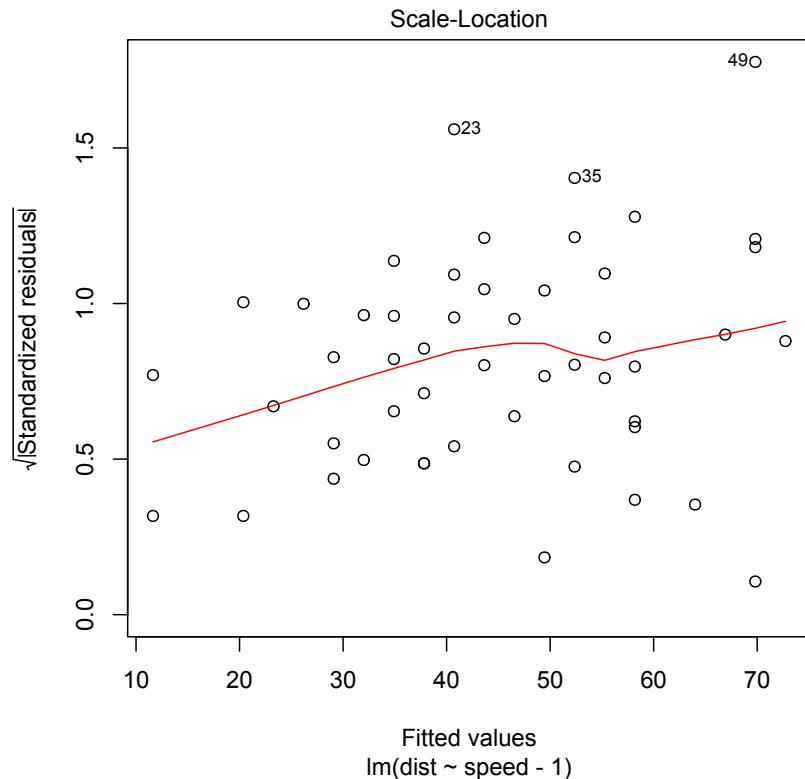
## 
## Call:
## lm(formula = dist ~ speed - 1, data = cars)
## 
## Residuals:
##      Min       1Q   Median       3Q      Max 
## -26.18  -12.64   -5.46    4.59   50.18 
## 
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## speed       2.909     0.141   20.6   <2e-16 ***
## ---      
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 16.3 on 49 degrees of freedom
## Multiple R-squared:  0.896, Adjusted R-squared:  0.894 
## F-statistic: 423 on 1 and 49 DF,  p-value: <2e-16
```

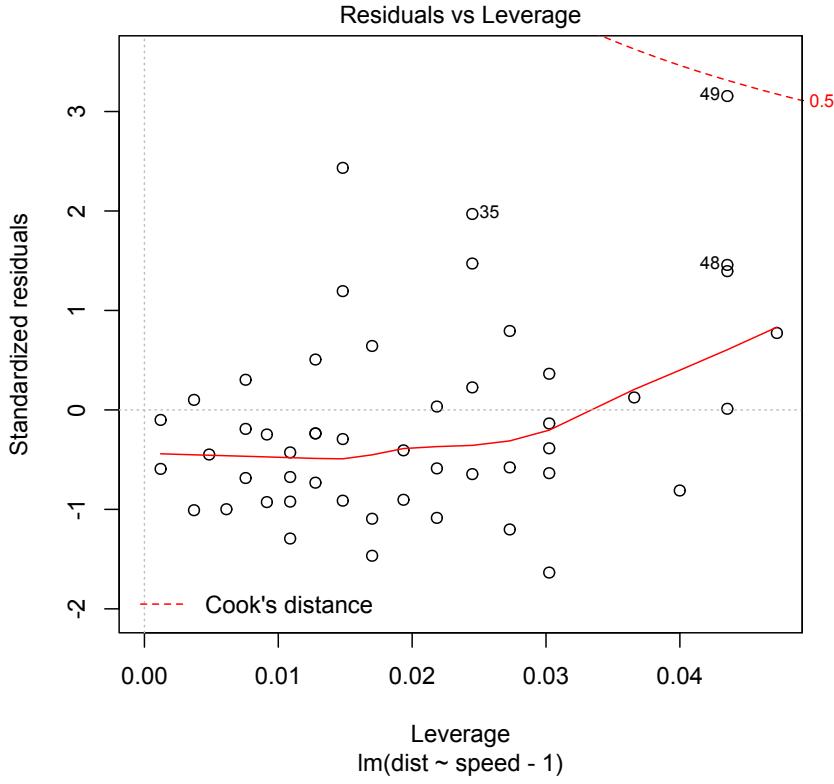
```
anova(fm2) # we calculate an ANOVA

## Analysis of Variance Table
##
## Response: dist
##              Df Sum Sq Mean Sq F value Pr(>F)
## speed         1 111949  111949     423 <2e-16 ***
## Residuals   49 12954    264
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```









We now we fit a second degree polynomial.

```
fm3 <- lm(dist ~ speed + I(speed^2), data=cars) # we fit a model, and then save the result
plot(fm3) # we produce diagnosis plots
summary(fm3) # we inspect the results from the fit

##
## Call:
## lm(formula = dist ~ speed + I(speed^2), data = cars)
##
## Residuals:
##      Min    1Q Median    3Q   Max 
## -28.72 -9.18 -3.19  4.63 45.15 
## 
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept)  2.470     14.817   0.17    0.87    
## speed        0.913      2.034   0.45    0.66    
## I(speed^2)    0.100      0.066   1.52    0.14    
## 
## Residual standard error: 15.2 on 47 degrees of freedom
## Multiple R-squared:  0.667, Adjusted R-squared:  0.653 
## F-statistic: 47.1 on 2 and 47 DF, p-value: 5.85e-12 

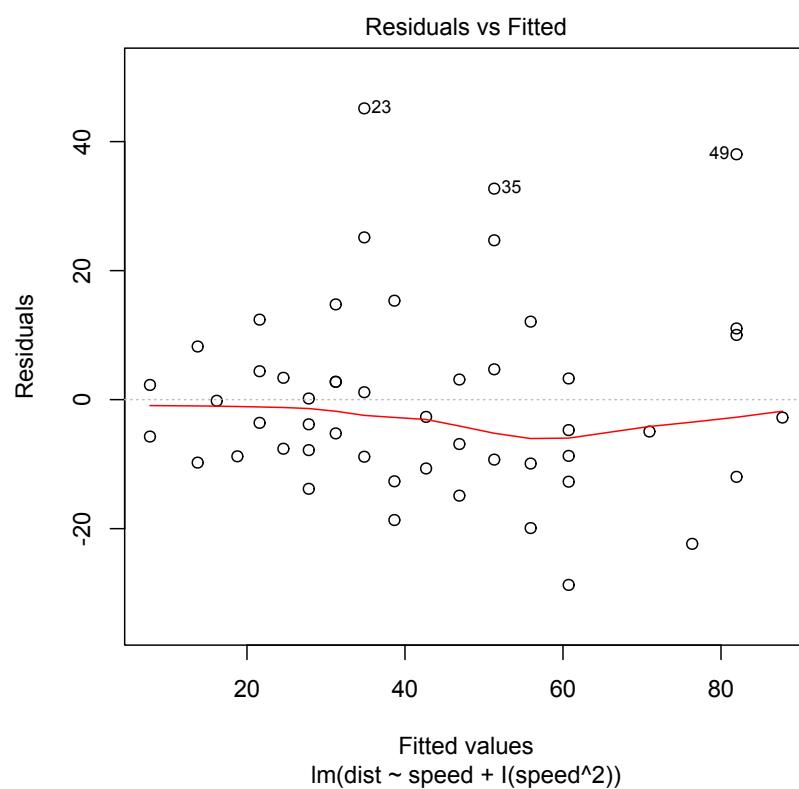
anova(fm3) # we calculate an ANOVA

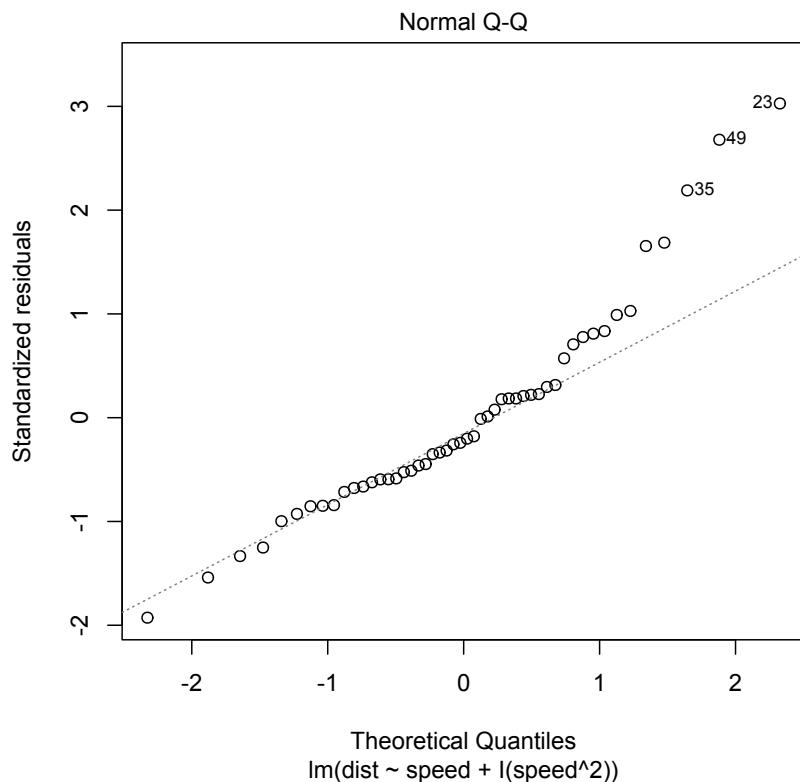
## Analysis of Variance Table
```

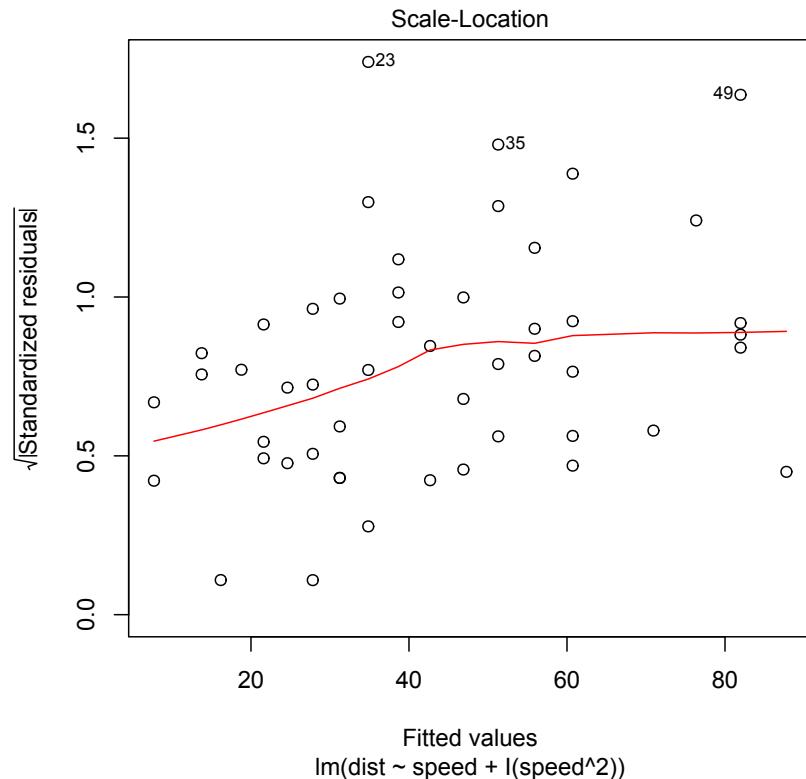
```

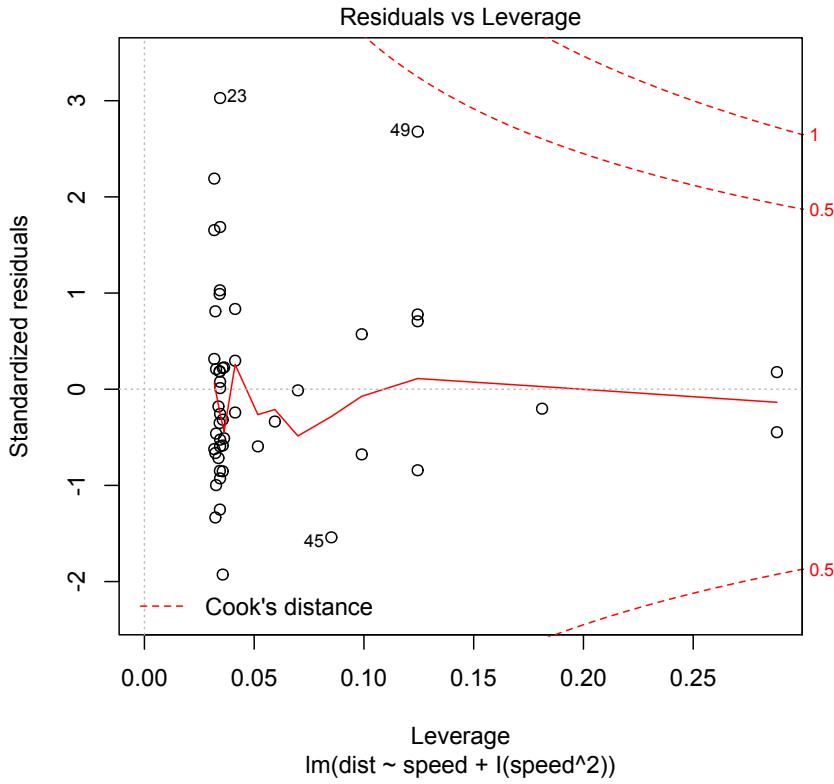
## 
## Response: dist
##           Df Sum Sq Mean Sq F value    Pr(>F)
## speed      1 21185  21185   92.0 1.2e-12 ***
## I(speed^2)  1    529     529     2.3   0.14
## Residuals  47 10825    230
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```









We can also compare the two models.

```
anova(fm2, fm1)

## Analysis of Variance Table
##
## Model 1: dist ~ speed - 1
## Model 2: dist ~ speed
##   Res.Df   RSS Df Sum of Sq    F Pr(>F)
## 1     49 12954
## 2     48 11354  1      1600 6.77  0.012 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Or three or more models. But be careful, as the order of the arguments matters.

```
anova(fm2, fm1, fm3)

## Analysis of Variance Table
##
## Model 1: dist ~ speed - 1
## Model 2: dist ~ speed
## Model 3: dist ~ speed + I(speed^2)
##   Res.Df   RSS Df Sum of Sq    F Pr(>F)
## 1     49 12954
```

```
## 2      48 11354  1      1600 6.95  0.011 *
## 3      47 10825  1      529 2.30  0.136
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We can use different criteria to choose the best model: significance based on  $P$ -values or information criteria (AIC, BIC) that penalize the result based on the number of parameters in the fitted model. In the case of AIC and BIC, a smaller value is better, and values returned can be either positive or negative, in which case more negative is better.

## B.8 Control of execution flow

### Conditional execution

#### Non-vectorized

R has two types of “if” statements, non-vectorized and vectorized. We will start with the non-vectorized one, which is similar to what is available in most other computer programming languages.

Before this we need to explain compound statements. Individual statements can be grouped into compound statements by enclosed them in curly braces.

```
print("A")
## [1] "A"
{
  print("B")
  print("C")
}
## [1] "B"
## [1] "C"
```

The example above is pretty useless, but becomes useful when used together with ‘control’ constructs. The `if` construct controls the execution of one statement, however, this statement can be a compound statement of almost any length or complexity. Play with the code below by changing the value assigned to `printing`, including NA, and logical(0).

```
printing <- TRUE
if (printing) {
  print("A")
  print("B")
}

## [1] "A"
## [1] "B"
```

The condition ‘( )’ can be anything yielding a logical vector, however, as this is not vectorized, only the first element will be used. Play with this example by changing the value assigned to `a`.

```
a <- 10.0
if (a < 0.0) print("a' is negative") else print("a' is not negative")

## [1] "'a' is not negative"

print("This is always printed")

## [1] "This is always printed"
```

As you can see above the statement immediately following `else` is executed if the condition is false. Later statements are executed independently of the condition.

Do you still remember the rules about continuation lines?

```
# 1
if (a < 0.0)
  print("a' is negative") else
  print("a' is not negative")
# 2 (not evaluated here)
if (a < 0.0) print("a' is negative")
else print("a' is not negative")
```

Why does only the second example above trigger an error?

Play with the use conditional execution, with both simple and compound statements, and also think how to combine `if` and `else` to select among more than two options.

There is in R a `switch` statement, that we will not describe here, that can be used to select among “cases”, or several alternative statements, based on an expression evaluating to a number or a character string.

Vectorized

The vectorized conditional execution is coded by means of a `function` called `ifelse` (one word). This function takes three arguments: a logical vector, a result vector for TRUE, a result vector for FALSE. All three can be any construct giving the necessary argument as their result. In the case of result vectors, recycling will apply if they are not of the correct length. **The length of the result is determined by the length of the logical vector in the first argument!**

```
a <- 1:10
ifelse(a > 5, 1, -1)

## [1] -1 -1 -1 -1 -1  1  1  1  1  1

ifelse(a > 5, a + 1, a - 1)

## [1]  0  1  2  3  4  7  8  9 10 11

ifelse(any(a>5), a + 1, a - 1) # tricky

## [1] 2

ifelse(logical(0), a + 1, a - 1) # even more tricky

## logical(0)

ifelse(NA, a + 1, a - 1) # as expected

## [1] NA
```

Try to understand what is going on in the previous example. Create your own examples to test how `ifelse` works.

Exercise: write using `ifelse` a single statement to combine numbers from `a` and `b` into a result vector `d`, based on whether the corresponding value in `c` is the character "a" or "b".

```
a <- rep(-1, 10)
b <- rep(+1, 10)
c <- c(rep("a", 5), rep("b", 5))
# your code
```

If you do not understand how the three vectors are built, or you cannot guess the values they contain by reading the code, print them, and play with the arguments, until you have clear what each parameter does.

### Why using vectorized functions and operators is important

If you have written programs in other languages, it would feel to you natural to use loops (`for`, `repeat` `while`, `repeat until`) for many of the things for which we have been using vectorization. When using the R language it is best to use vectorization whenever possible, because it keeps the listing of scripts and programs shorter and easier to understand (at least for those with experience in R). However, there is another very important reason: execution speed. The reason behind this is that R is an interpreted language. In current versions of R it is possible to byte-compile functions, but this is rarely used for scripts, and even byte-compiled loops are much slower and vectorized functions.

However, there are cases where we need to repeatedly execute statements in a way that cannot be vectorized, or when we do not need to maximize execution speed. The R language does have loop constructs, and we will describe them next.

### Repetition

The most frequently used type of loop is a `for` loop. These loops work in R are based on lists or vectors of values to act upon.

```
b <- 0
for (a in 1:5) b <- b + a
b
## [1] 15

b <- sum(1:5) # built-in function
b
## [1] 15
```

Here the statement `b <- b + a` is executed five times, with `a` sequentially taking each of the values in `1:5`. Instead of a simple statement used here, also a compound statement could have been used.

Here are a few examples that show some of the properties of `for` loops and functions, combined with the use of a function.

```

test.for <- function(x) {
  for (i in x) {print(i)}
}
test.for(numeric(0))
test.for(1:3)

## [1] 1
## [1] 2
## [1] 3

test.for(NA)

## [1] NA

test.for(c("A", "B"))

## [1] "A"
## [1] "B"

test.for(c("A", NA))

## [1] "A"
## [1] NA

test.for(list("A", 1))

## [1] "A"
## [1] 1

test.for(c("z", letters[1:4]))

## [1] "z"
## [1] "a"
## [1] "b"
## [1] "c"
## [1] "d"

```

In contrast to other languages, in R function arguments are not checked for ‘type’ when the function is called. The only requirement is that the function code can handle the argument provided. In this example you can see that the same function works with numeric and character vectors, and with lists. We haven’t seen lists before. As earlier discussed all elements in a vector should have the same type. This is not the case for lists. It is also interesting to note that a list or vector of length zero is a valid argument, that triggers no error, but that as one would expect, causes the statements in the loop body to be skipped.

Some examples of use of `for` loops — and of how to avoid there use.

```

a <- c(1, 4, 3, 6, 8)
for(x in a) x*x # result is lost
for(x in a) print(x*x) # print is needed!

## [1] 2
## [1] 8
## [1] 6
## [1] 12

```

```

## [1] 16

b <- for(x in a) x*2 # doesn't work as expected, but triggers no error
b

## NULL

for(x in a) b <- x*2 # a bit of a surprise, as b is not a vector!
b

## [1] 16

for(i in seq(along=a)) {
  b[i] <- a[i]^2
  print(b)
}

## [1] 1
## [1] 1 16
## [1] 1 16 9
## [1] 1 16 9 36
## [1] 1 16 9 36 64

b # is a vector!

## [1] 1 16 9 36 64

# a bit faster if we first allocate a vector of the required length
b <- numeric(length(a))
for(i in seq(along=a)) {
  b[i] <- a[i]^2
  print(b)
}

## [1] 1 0 0 0 0
## [1] 1 16 0 0 0
## [1] 1 16 9 0 0
## [1] 1 16 9 36 0
## [1] 1 16 9 36 64

b # is a vector!

## [1] 1 16 9 36 64

# vectorization is simplest and fastest
b <- a^2
b

## [1] 1 16 9 36 64

```

Look at the results from the above examples, and try to understand where does the returned value come from in each case.

We sometimes may not be able to use vectorization, or may be easiest to not use it. However, whenever working with large data sets, or many similar datasets, we will need to take performance into account. As vectorization usually also makes code simpler, it is good style to use it whenever possible.

```

b <- numeric(length(a)-1)
for(i in seq(along=b)) {
  b[i] <- a[i+1] - a[i]
  print(b)
}

## [1] 3 0 0 0
## [1] 3 -1 0 0
## [1] 3 -1 3 0
## [1] 3 -1 3 2

# although in this case there were alternatives, there
# are other cases when we need to use indexes explicitly
b <- a[2:length(a)] - a[1:length(a)-1]
b

## [1] 3 -1 3 2

# or even better
b <- diff(a)
b

## [1] 3 -1 3 2

```

`seq(along=b)` builds a new numeric vector with a sequence of the same length as the length as the vector given as argument for parameter ‘along’.

`while` loops are quite frequently also useful. Instead of a list or vector, they take a logical argument, which is usually an expression, but which can also be a variable. For example the previous calculation could be also done as follows.

```

a <- c(1, 4, 3, 6, 8)
i <- 1
while (i < length(a)) {
  b[i] <- a[i]^2
  print(b)
  i <- i + 1
}

## [1] 1 -1 3 2
## [1] 1 16 3 2
## [1] 1 16 9 2
## [1] 1 16 9 36

b

## [1] 1 16 9 36

```

Here is another example. In this case we use the result of the previous iteration in the current one. In this example you can also see, that it is allowed to put more than one statement in a single line, in which case the statements should be separated by a semicolon ( ; ).

```

a <- 2
while (a < 50) {print(a); a <- a^2}

```

```
## [1] 2
## [1] 4
## [1] 16

print(a)

## [1] 256
```

Make sure that you understand why the final value of `a` is larger than 50. `repeat` is seldom used, but adds flexibility as `break` can be in the middle of the compound statement.

```
a <- 2
repeat{
  print(a)
  a <- a^2
  if (a > 50) {print(a); break()}
}

## [1] 2
## [1] 4
## [1] 16
## [1] 256

# or more elegantly
a <- 2
repeat{
  print(a)
  if (a > 50) break()
  a <- a^2
}

## [1] 2
## [1] 4
## [1] 16
## [1] 256
```

Please, make sure you understand what is happening in the previous examples.

## Nesting

All the execution-flow control statements seen above can be nested. We will show an example with two `for` loops. We first need a matrix of data to work with:

```
A <- matrix(1:50, 10)
A

##      [,1] [,2] [,3] [,4] [,5]
## [1,]     1    11   21   31   41
## [2,]     2    12   22   32   42
## [3,]     3    13   23   33   43
## [4,]     4    14   24   34   44
## [5,]     5    15   25   35   45
## [6,]     6    16   26   36   46
```

```

## [7,]    7   17   27   37   47
## [8,]    8   18   28   38   48
## [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, 10, 5)
A

##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1   11   21   31   41
## [2,]    2   12   22   32   42
## [3,]    3   13   23   33   43
## [4,]    4   14   24   34   44
## [5,]    5   15   25   35   45
## [6,]    6   16   26   36   46
## [7,]    7   17   27   37   47
## [8,]    8   18   28   38   48
## [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

# argument names used for clarity
A <- matrix(1:50, nrow = 10)
A

##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1   11   21   31   41
## [2,]    2   12   22   32   42
## [3,]    3   13   23   33   43
## [4,]    4   14   24   34   44
## [5,]    5   15   25   35   45
## [6,]    6   16   26   36   46
## [7,]    7   17   27   37   47
## [8,]    8   18   28   38   48
## [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, ncol = 5)
A

##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1   11   21   31   41
## [2,]    2   12   22   32   42
## [3,]    3   13   23   33   43
## [4,]    4   14   24   34   44
## [5,]    5   15   25   35   45
## [6,]    6   16   26   36   46
## [7,]    7   17   27   37   47
## [8,]    8   18   28   38   48
## [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, nrow = 10, ncol = 5)
A

##      [,1] [,2] [,3] [,4] [,5]
## [1,]    1   11   21   31   41
## [2,]    2   12   22   32   42
## [3,]    3   13   23   33   43
## [4,]    4   14   24   34   44
## [5,]    5   15   25   35   45

```

```
## [6,]    6   16   26   36   46
## [7,]    7   17   27   37   47
## [8,]    8   18   28   38   48
## [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50
```

All the statements above are equivalent, but some are easier to read than others.

```
row.sum <- numeric() # slower as size needs to be expanded
for (i in 1:nrow(A)) {
  row.sum[i] <- 0
  for (j in 1:ncol(A))
    row.sum[i] <- row.sum[i] + A[i, j]
}
print(row.sum)

## [1] 105 110 115 120 125 130 135 140 145 150
```

```
row.sum <- numeric(nrow(A)) # faster
for (i in 1:nrow(A)) {
  row.sum[i] <- 0
  for (j in 1:ncol(A))
    row.sum[i] <- row.sum[i] + A[i, j]
}
print(row.sum)

## [1] 105 110 115 120 125 130 135 140 145 150
```

Look at the output of these two examples to understand what is happening differently with `row.sum`.

The code above is very general, it will work with any size of two dimensional matrix, which is good programming practice. However, sometimes we need more specific calculations. `A[1, 2]` selects one cell in the matrix, the one on the first row of the second column. `A[1, ]` selects row one, and `A[, 2]` selects column two. In the example above the value of `i` changes for each iteration of the outer loop. The value of `j` changes for each iteration of the inner loop, and the inner loop is run in full for each iteration of the outer loop. The inner loop index `j` changes fastest.

Exercises: 1) modify the example above to add up only the first three columns of `A`, 2) modify the example above to add the last three columns of `A`.

Will the code you wrote continue working as expected if the number of rows in `A` changed? and what if the number of columns in `A` changed, and the required results still needed to be calculated for relative positions? What would happen if `A` had fewer than three columns? Try to think first what to expect based on the code you wrote. Then create matrices of different sizes and test your code. After that think how to improve the code, at least so that wrong results are not produced.

Vectorization can be achieved in this case easily for the inner loop.

```

row.sum <- numeric(nrow(A)) # faster
for (i in 1:nrow(A)) {
  row.sum[i] <- sum(A[i, ])
}
print(row.sum)

## [1] 105 110 115 120 125 130 135 140 145 150

```

`A[i, ]` selects row `i` and all columns. In R, the row index always comes first, which is not the case in all programming languages.

Full vectorization can be achieved with `apply` functions.

```

row.sum <- apply(A, MARGIN = 1, sum) # MARGIN=1 indicates rows
print(row.sum)

## [1] 105 110 115 120 125 130 135 140 145 150

```

How would you change this last example, so that only the last three columns are added up? (Think about use of subscripts to select a part of the matrix.)

There are many variants of `apply` functions, both in base R and in contributed packages.

## B.9 Packages

In R speak ‘library’ is the location where ‘packages’ are installed. Packages are sets of functions, and data, specific for some particular purpose, that can be loaded into an R session to make them available so that they can be used in the same way as built-in R functions and data. The function `library` is used to load packages, already installed in the local R library, into the current session, while the function `install.packages` is used to install packages, either from a file, or directly from the internet into the library. When using RStudio it is easiest to use RStudio commands (which call `install.packages` and `update.packages`) to install and update packages.

```
library(graphics)
```

Currently there are thousands of packages available. The most reliable source of packages is CRAN, as only packages that pass strict tests and are actively maintained are included. In some cases you may need or want to install less stable code, and this is also possible.

R packages can be installed either from source, or from already built ‘binaries’. Installing from sources, depending on the package, may require quite a lot of additional software to be available. Under MS-Windows, very rarely the needed shell, commands and compilers are already available. Installing then is not too difficult (you will need RTools, and MiKTeX). For this reason it is the norm to install packages from binary .zip files. Under Linux most tools will be available, or very easy to install, so it is not unusual to install from sources. For OS X (Mac) the situation is somewhere in-between. If the tools are available, packages can be very easily installed from source from within RStudio.

The development of packages is beyond the scope of the current course, but it is still interesting to know a few things about packages. Using RStudio it is relatively easy to develop your own packages. Packages can be of very different sizes. Packages use a relatively rigid structure of folder for storing the different types of files, and there is a built-in help system, that one needs to use, so that the package documentation gets linked to the R help system when the package is loaded. In addition to R code, packages can call C, C++, FORTRAN, Java, etc. functions and routines, but some kind of ‘glue’ is needed, as data is stored differently. At least for C++, the recently developed Rcpp R package makes the gluing extremely easy.

In addition to some packages from CRAN, later in the course we will use a suite of packages for photobiology that I have developed during the last couple of years. Some of the functions in these packages are very simple, and others more complex. In one of the packages, I included some C++ functions to improve performance. Replacing some R for loops with C++ for loops and iterators, resulted in a huge speed increase. The reason for this is that R is an interpreted language and C++ is compiled into machine code. Recent versions of R allow byte-compilation which can give some speed improvement, without need to switch to another language.

The source code for the photobiology and many other packages is freely available, so if you are interested you can study it. For any function defined in R, typing at the command prompt the name of the function without the parentheses lists the code.

```
length # a function defined in C within R itself
## function (x) .Primitive("length")
SEM # the function we defined earlier
## function(x, na.rm=FALSE){sqrt(var(x, na.rm=na.rm)/length(na.omit(x)))}
```

One good way of learning how R works, is by experimenting with it, and whenever using a certain function looking at the help, to check what are all the available options.



## Making publication quality plots with R

### C.1 Packages used in this chapter

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

```
library(ggplot2)
library(scales)
library(ggtern)
library(ggmap)
library(rgdal)

## Error: there is no package called 'rgdal'

library(Hmisc)

## Error: there is no package called 'Hmisc'

library(plyr)
library(grid)
library(photobiologygg)
```

### C.2 Introduction

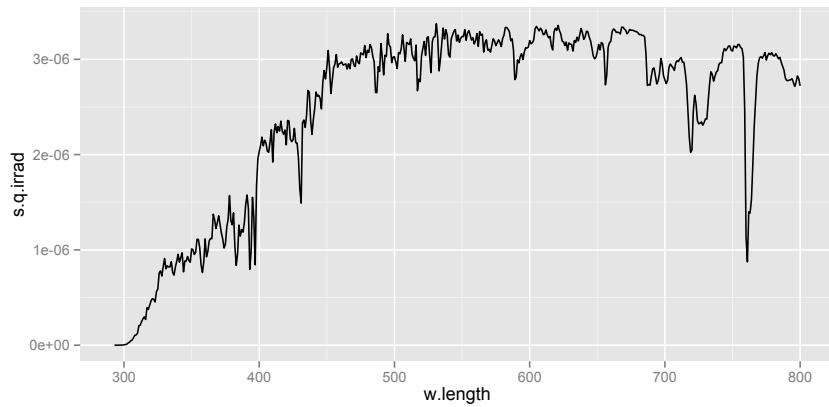
Being R extensible, in addition to the built-in plotting functions, there are several alternatives provided by packages. Of the general purpose ones, the most extensively used are *Lattice* and *ggplot2*. There are packages that add extra functionality to these packages.

In the examples in this handbook we mainly use *ggplot*, *ggmap* and *ggtern*, together with our own *photobiologygg*. In this appendix we give a very brief introduction to the ‘grammar of graphics’ and *ggplot2*.

### C.3 Bases of plotting with `ggplot2`

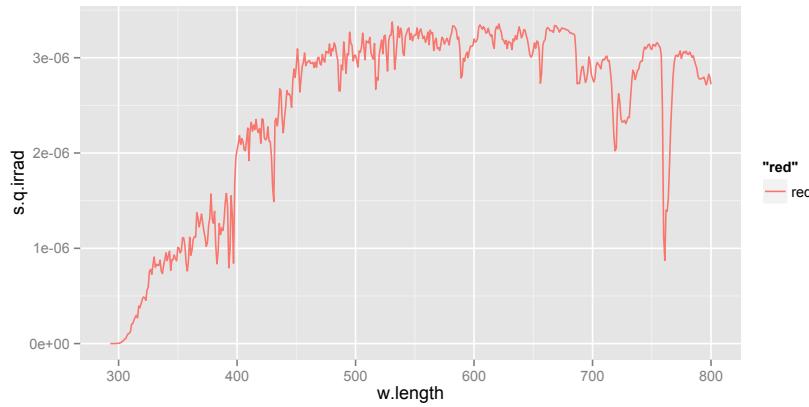
The grammar of graphics is based on aesthetics (`aes`) as for example colour, geometric elements `geom_...` such as lines, and points, statistics `stat_...`, scales `scale_...`, labels `labs`, and themes `theme_...`. Plots are assembled from these elements, we start with a plot with two aesthetics, and one geom:

```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line()
```



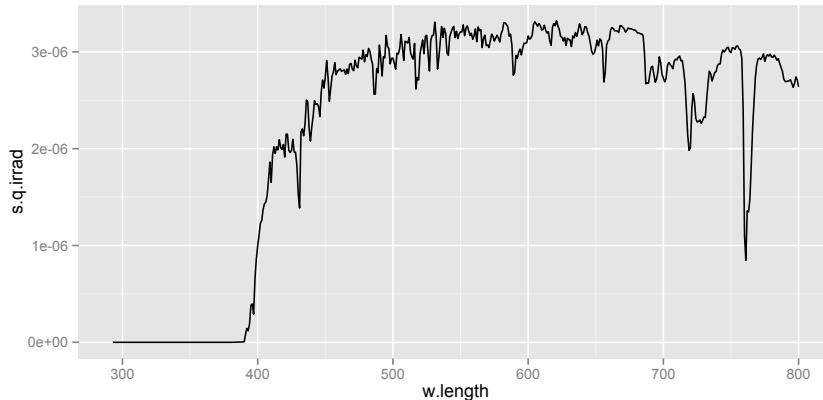
Aesthetics can be ‘assigned’ to data variables, and to constants:

```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad, colour="red")) +
  geom_line()
```



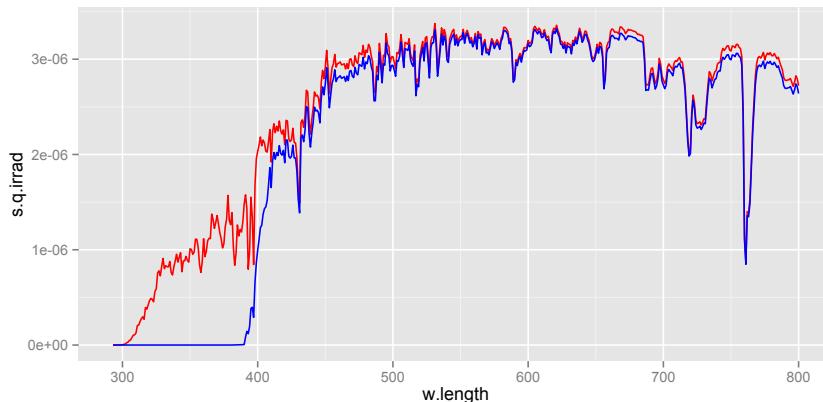
Data can be the ‘result of a calculation’:

```
ggplot(sun.dt * gg400.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line()
```



The aesthetics and data given as `ggplot`'s arguments become the defaults for the geoms, but geoms also take aesthetics and data as arguments, which then override the defaults:

```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line(colour="red") +
  geom_line(data=sun.dt * gg400.dt, colour="blue")
```



Another way of plotting these data, is to first assemble a single `data.frame` or `data.table` with all the data. We will use the example data that is as `data.tables`:

```
unfiltered_sun.dt <- copy(sun.dt)
unfiltered_sun.dt[ , filter := "none"]

##      w.length s.e.irrad s.q.irrad filter
## 1:      293 2.610e-06 6.392e-12   none
## 2:      294 6.142e-06 1.510e-11   none
## 3:      295 2.176e-05 5.366e-11   none
## 4:      296 6.780e-05 1.678e-10   none
## 5:      297 1.533e-04 3.807e-10   none
##  ---
## 504:     796 4.081e-01 2.715e-06   none
## 505:     797 4.141e-01 2.759e-06   none
## 506:     798 4.236e-01 2.826e-06   none
## 507:     799 4.186e-01 2.796e-06   none
## 508:     800 4.069e-01 2.721e-06   none
```

```

filtered_sun.dt <- sun.dt * gg400.dt
filtered_sun.dt[ , filter := "GG400"]

##      w.length s.e.irrad s.q.irrad filter
## 1:      293 2.610e-11 6.392e-17 GG400
## 2:      294 6.142e-11 1.510e-16 GG400
## 3:      295 2.176e-10 5.366e-16 GG400
## 4:      296 6.780e-10 1.678e-15 GG400
## 5:      297 1.533e-09 3.807e-15 GG400
##   --
## 504:     796 3.958e-01 2.634e-06 GG400
## 505:     797 4.017e-01 2.676e-06 GG400
## 506:     798 4.109e-01 2.741e-06 GG400
## 507:     799 4.060e-01 2.712e-06 GG400
## 508:     800 3.947e-01 2.639e-06 GG400

data4plot.dt <- rbind(unfiltered_sun.dt, filtered_sun.dt)
data4plot.dt[ , filter := factor(filter)]

##      w.length s.e.irrad s.q.irrad filter
## 1:      293 2.610e-06 6.392e-12 none
## 2:      294 6.142e-06 1.510e-11 none
## 3:      295 2.176e-05 5.366e-11 none
## 4:      296 6.780e-05 1.678e-10 none
## 5:      297 1.533e-04 3.807e-10 none
##   --
## 1012:     796 3.958e-01 2.634e-06 GG400
## 1013:     797 4.017e-01 2.676e-06 GG400
## 1014:     798 4.109e-01 2.741e-06 GG400
## 1015:     799 4.060e-01 2.712e-06 GG400
## 1016:     800 3.947e-01 2.639e-06 GG400

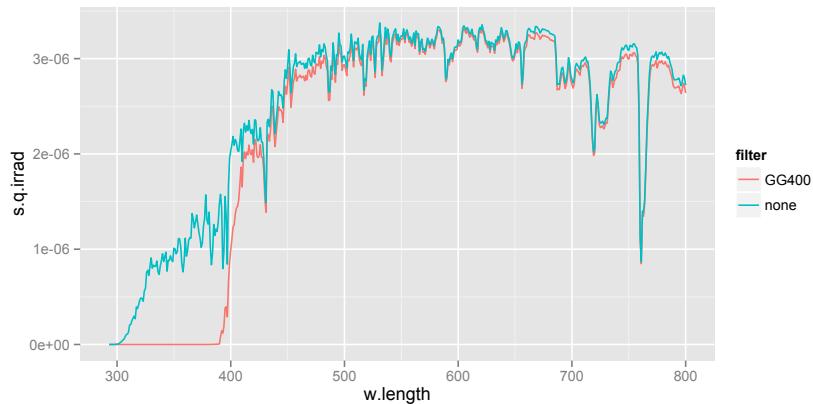
```

Now we can do the plot assigning `filter` to an aesthetic:

```

ggplot(data4plot.dt, aes(x=w.length, y=s.q.irrad, colour=filter)) +
  geom_line()

```

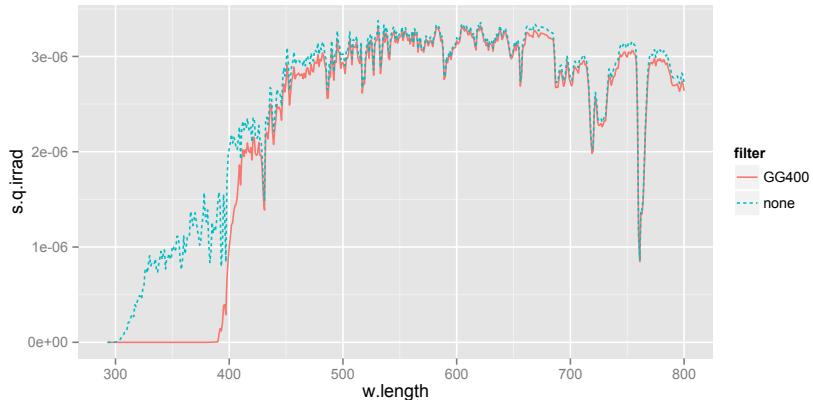


We can assign the same variable to more than one aesthetic:

```

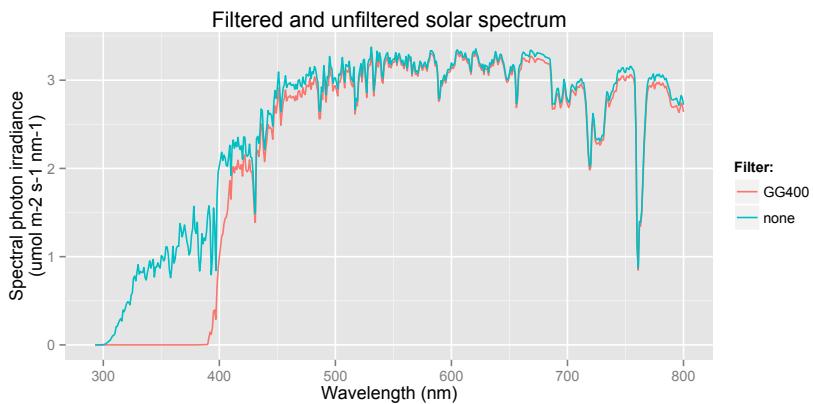
ggplot(data4plot.dt, aes(x=w.length, y=s.q.irrad,
                           colour=filter, linetype=filter)) +
  geom_line()

```



We can change the labels for the different aesthetics, and give a title:

```
ggplot(data4plot.dt,
       aes(x=w.length, y=s.q.irrad * 1e6, colour=filter)) +
  geom_line() +
  labs(x="Wavelength (nm)",
       y="Spectral photon irradiance\n(umol m-2 s-1 nm-1)",
       colour="Filter:",
       title="Filtered and unfiltered solar spectrum")
```

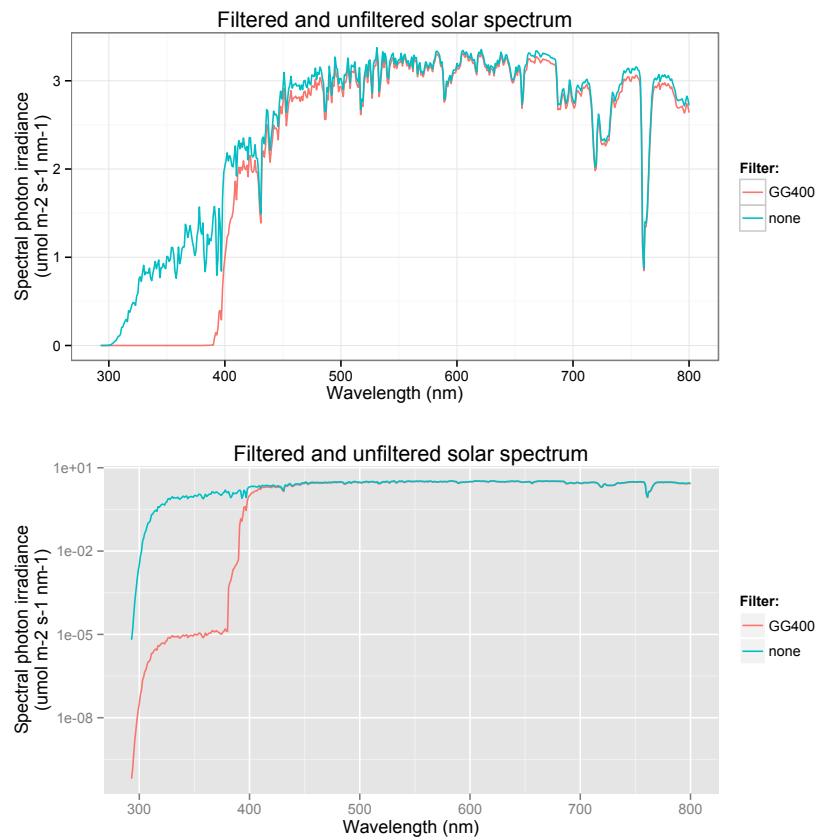


We can assign a ggplot object to a variable:

```
myplot <- ggplot(data4plot.dt,
                   aes(x=w.length, y=s.q.irrad * 1e6, colour=filter)) +
  geom_line() +
  labs(x="Wavelength (nm)",
       y="Spectral photon irradiance\n(umol m-2 s-1 nm-1)",
       colour="Filter:",
       title="Filtered and unfiltered solar spectrum")
```

And now we can add more elements to the plot stored in the variable:

```
myplot + theme_bw()
myplot + scale_y_log10()
```

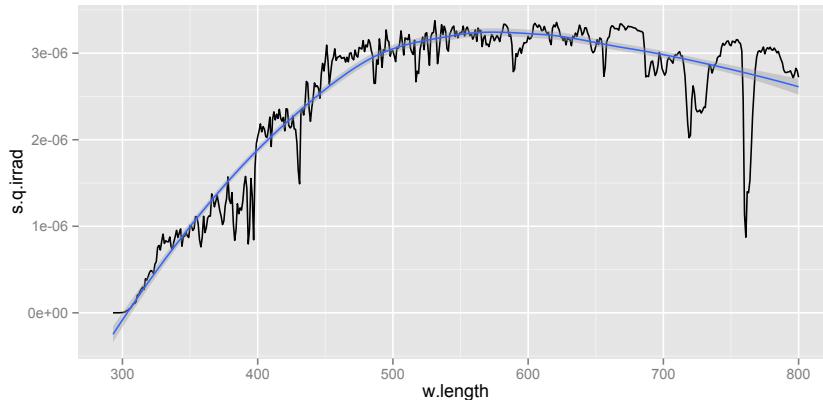


#### C.4 Adding fitted curves, including splines

We will now show an example of use of `stat_smooth` using the default spline smoothing.

```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line() +
  stat_smooth()

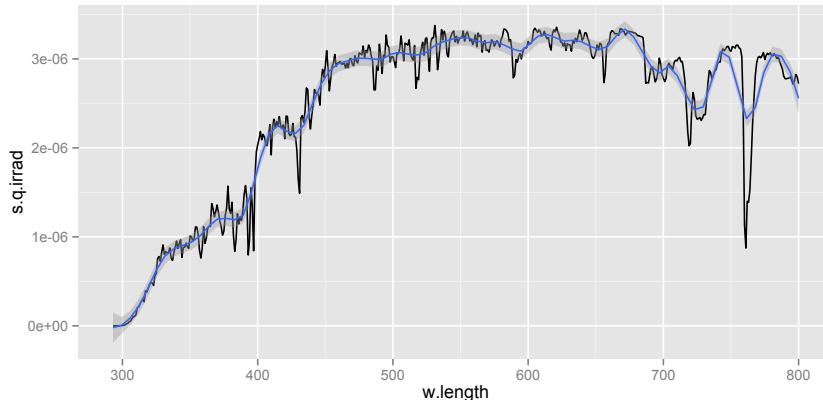
## geom_smooth: method="auto" and size of largest group is
<1000, so using loess. Use 'method = x' to change the smoothing
method.
```



By adjusting one of its parameters, `span`, we make the spline more “flexible”:

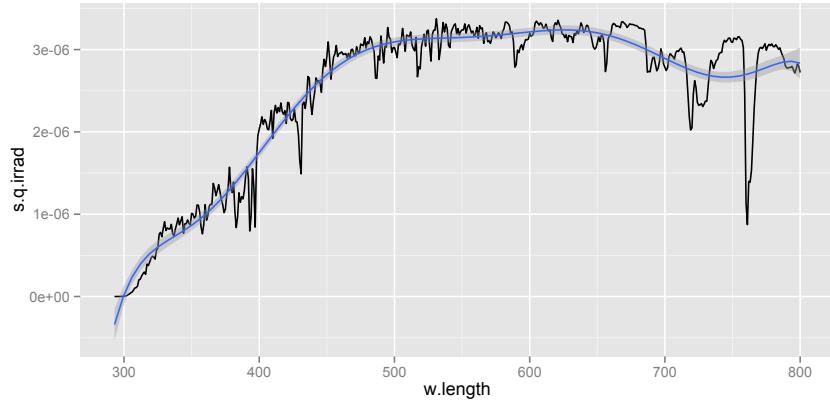
```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line() +
  stat_smooth(span=0.1)

## geom_smooth: method="auto" and size of largest group is
<1000, so using loess. Use 'method = x' to change the smoothing
method.
```



Instead of using the default spline, we can use a linear model fit. In this example we use a polynomial of order 8, fitted by lm, as smoother:

```
ggplot(sun.dt, aes(x=w.length, y=s.q.irrad)) +
  geom_line() +
  stat_smooth(method="lm", formula=y~poly(x, 8))
```



It is possible to use other types of models, including GAM and GLM, as smoothers, but we will not give examples of the use these more advanced models.

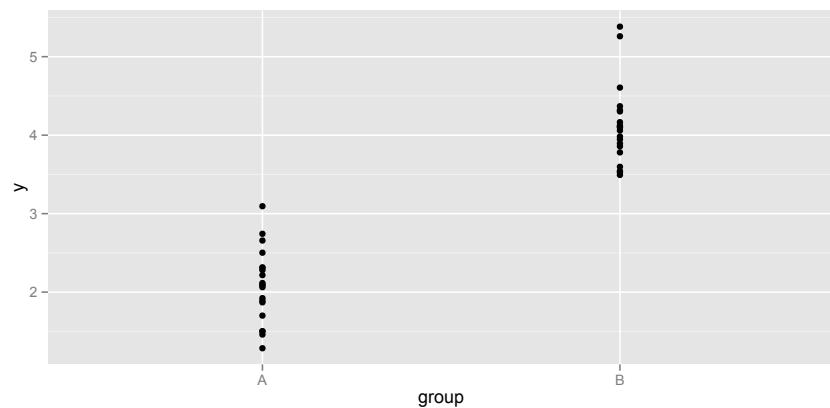
### C.5 Adding statistical “summaries”

It is also possible to summarize data on-the-fly when plotting, but before showing this we will generate some normally distributed artificial data:

```
fake.data <- data.frame(
  y = c(rnorm(20, mean=2, sd=0.5), rnorm(20, mean=4, sd=0.7)),
  group = factor(c(rep("A", 20), rep("B", 20)))
)
```

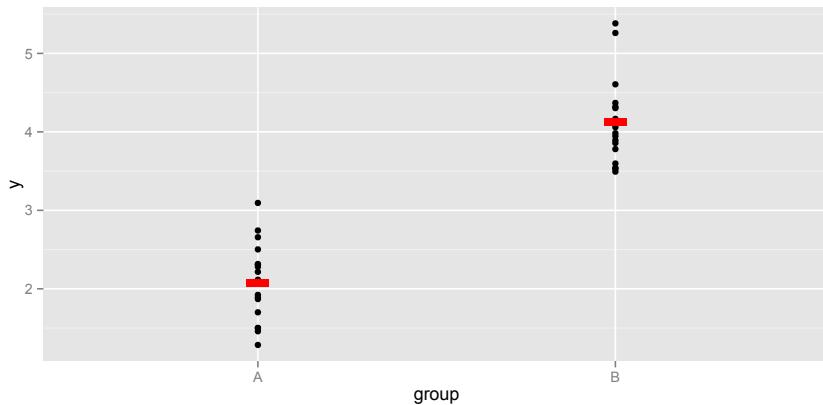
Now we use these data to plot means and confidence intervals by group:

```
fig2 <- ggplot(data=fake.data, aes(y=y, x=group)) + geom_point()
```

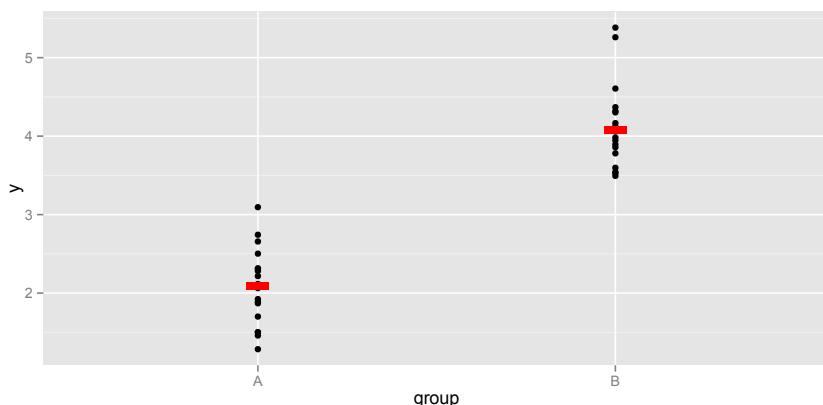


We have saved the base figure in `fig2`, so now we can play with different summaries. We first add just the mean. In this case we need to add as argument to `stat_summary` the geom to use, as the default one expects data for plotting error bars, in later examples, this is not needed.

```
fig2 + stat_summary(fun.y = "mean", geom="point",
                    colour="red", shape="-", size=20)
```



```
fig2 + stat_summary(fun.y = "median", geom="point",
                    colour="red", shape="-", size=20)
```



We can add the means and  $p = 0.95$  confidence intervals not assuming normality (using the actual distribution of the data by bootstrapping):

```
fig2 + stat_summary(fun.data = "mean_cl_boot",
                    colour="red", size=1, alpha=0.7)
```

```
## Error: Hmisc package required for this functionality.
Please install and try again.
```

We can instead add the means and  $p = 0.90$  confidence intervals, by supplying a value to parameter `conf.int`:

```
fig2 + stat_summary(fun.data = "mean_cl_boot", conf.int=0.90,
                    colour="red", size=1, alpha=0.7)
```

```
## Error: Hmisc package required for this functionality.
Please install and try again.
```

We can add the mean and  $p = 0.95$  confidence intervals assuming normality (using the  $t$  distribution):

```
fig2 + stat_summary(fun.data = "mean_cl_normal",
                    colour="red", size=1, alpha=0.7)

## Error: Hmisc package required for this functionality.
Please install and try again.
```

In this case the multiplier `mult` is by default calculated from the  $t$  distribution according to degrees of freedom, but if we force the multiplier to 1, then we get error bars corresponding to  $\pm$ s.e. (standard errors).

```
fig2 + stat_summary(fun.data = "mean_cl_normal", mult=1,
                    colour="red", size=1, alpha=0.7)

## Error: Hmisc package required for this functionality.
Please install and try again.
```

Finally we can plot error bars showing  $\pm$ s.d. (standard deviation). The default value for `mult` is 2, giving error bars  $\pm 2$  s.d., we use 1 as multiplier instead.

```
fig2 + stat_summary(fun.data = "mean_sdl",
                    colour="red", size=1, alpha=0.7)

## Error: Hmisc package required for this functionality.
Please install and try again.
```

We do not show it here, but instead of using these functions (from package Hmisc) it is possible to define one's own functions.

Finally we plot the means in a bar plot, with the observations superimposed and  $p = 0.95$  C.I. (the order in which the geoms are added is important: by having `geom_point` last it is plotted on top of the bars. In this case we set `fill`, `colour` and `alpha` (transparency) to constants, but in more complex data sets they can be assigned to factors in the data set.

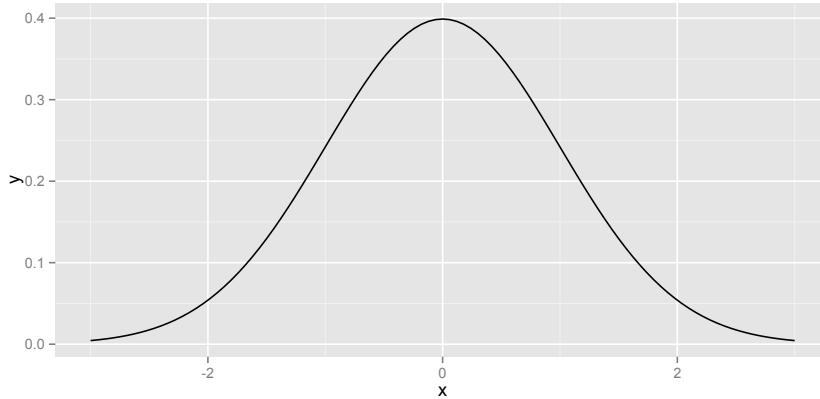
```
ggplot(data=fake.data, aes(y=y, x=group)) +
  stat_summary(fun.y = "mean", geom = "bar",
              fill="yellow", colour="black") +
  stat_summary(fun.data = "mean_cl_normal",
              geom = "errorbar",
              width=0.1, size=1, colour="red") +
  geom_point(size=3, alpha=0.3)

## Error: Hmisc package required for this functionality.
Please install and try again.
```

## C.6 Plotting functions

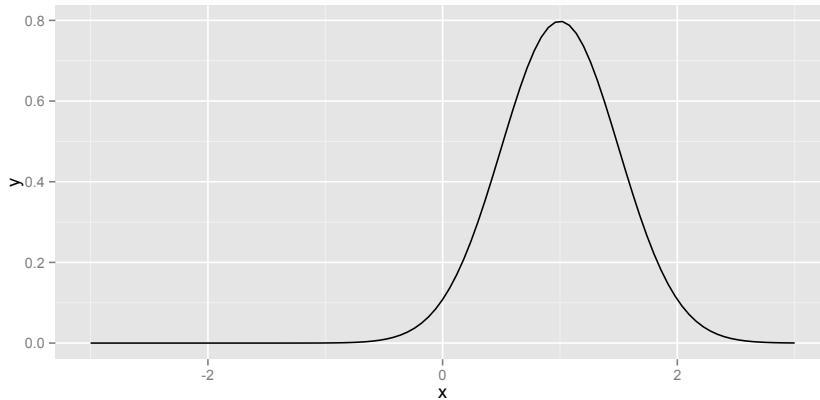
We can also directly plot functions, without need to generate data beforehand:

```
ggplot(data.frame(x=-3:3), aes(x=x)) +
  stat_function(fun=dnorm)
```



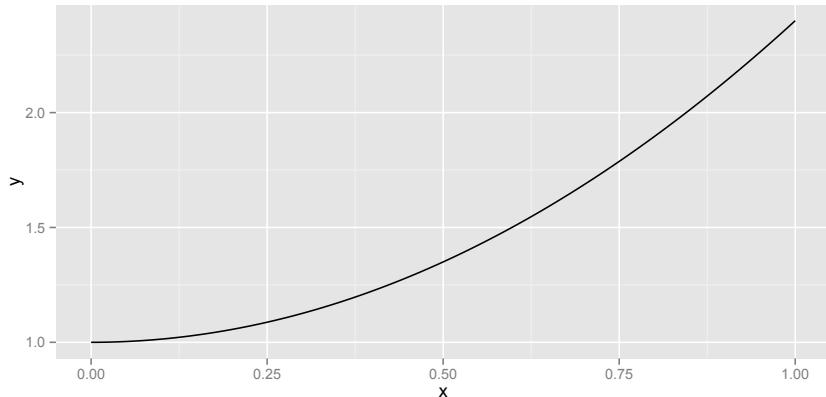
We can even pass additional arguments to a function:

```
ggplot(data.frame(x=-3:3), aes(x=x)) +
  stat_function(fun = dnorm, args = list(mean = 1, sd = .5))
```



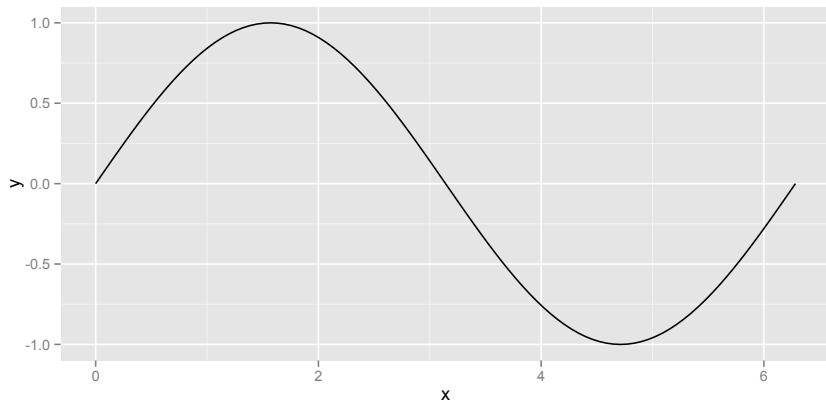
Of course, user-defined functions (not shown), and anonymous functions can also be used:

```
ggplot(data.frame(x=0:1), aes(x=x)) +
  stat_function(fun = function(x, a, b){a + b * x^2},
                args = list(a = 1, b = 1.4))
```



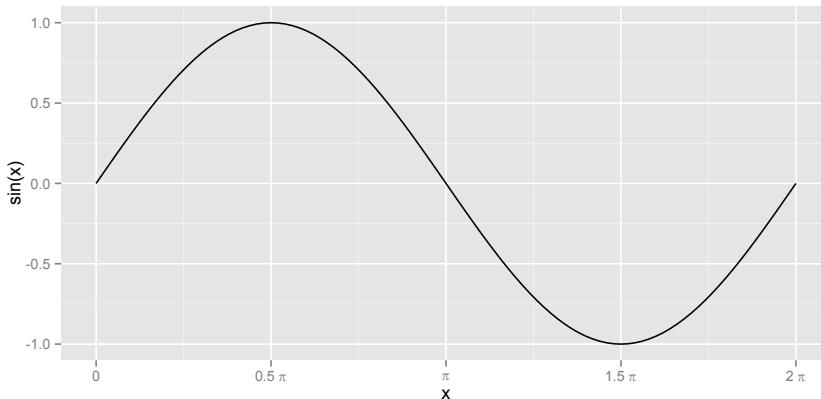
Here is another example of a predefined function, but in this case the default scale is not the best:

```
ggplot(data.frame(x=c(0, 2 * pi)), aes(x=x)) +
  stat_function(fun=sin)
```



In this case we need to change the x-axis scale to better suit the sin function and the use of radians as angular units:

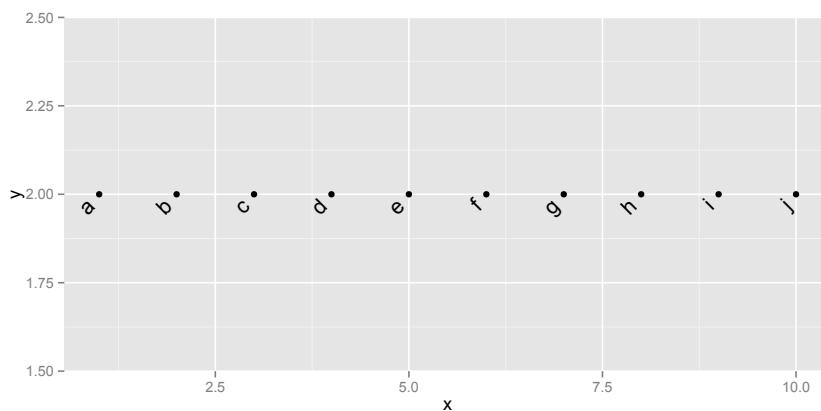
```
ggplot(data.frame(x=c(0, 2 * pi)), aes(x=x)) +
  stat_function(fun=sin) +
  scale_x_continuous(
    breaks=c(0, 0.5, 1, 1.5, 2) * pi,
    labels=c("0", expression(0.5~pi), expression(pi),
            expression(1.5~pi), expression(2~pi))) +
  labs(y="sin(x)")
```



## C.7 Plotting text

One can use `geom_text` to add text labels to observations. The aesthetic `label` gives text and the usual aesthetics `x` and `y` the location of the labels. As one would expect the `colour` aesthetic can be also used for text. In addition `angle` and `vjust` and `hjust` can be used to rotate the label, and adjust its position. The default value of zero for both `hjust` and `vjust` centres the label. The centre of the text is at the supplied `x` and `y` coordinates. ‘Vertical’ and ‘horizontal’ for justification refer to the text, not the plot. This is important when `angle` is different from zero. Negative justification values, shift the label left or down, and positive values right or up. A value of 1 or -1 sets the text so that its edge is at the supplied coordinate. Values outside the range -1...1 sift the text even further away.

```
my.data <- data.frame(x=1:10, y=rep(2, 10), label=paste(letters[1:10], " "))
ggplot(my.data, aes(x,y,label=label)) + geom_text(angle=45, hjust=1) + geom_point()
```



In this example we use `paste` (which uses recycling here) to add a space at the end of each label. Justification values outside the range -1...1 are allowed, but are relative to the width of the label. As the default font used in this case has variable widths with characters, the justification would be inconsistent (e.g. try the

code above but using `hjust` set to 3 instead of to 1 without pasting a space character to the labels.)

## C.8 Scales

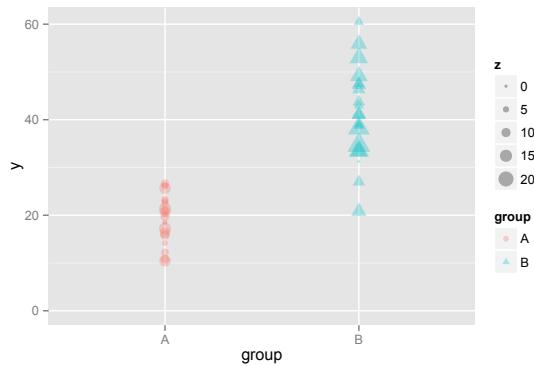
Scales map data onto aesthetics. There are different types of scales depending on the characteristics of the data being mapped: scales can be continuous or discrete. And of course, there are scales for different attributes of the plotted object, such as `colour`, `size`, `posititon` (`x`, `y`, `z`), `alpha` or transparency, `angle`, `justification`, etc. This means that many properties of, for example, the symbols used in a plot can be either set by a constant, or mapped to data. The most elemental mapping is `identity`, which means that the data is taken at its face value. In a numerical scale, say `scale_x_continuous`, this means that for example a '5' in the data is plotted at a position in the plot corresponding to the value '5' along the x-axis. A simple mapping could be a `log10` transformation, that we can easily achieve with the pre-defined `scale_x_log10` in which case the position on the x-axis will be based on the logarithm of the original data. A continuous data variable can, if we think it useful for describing our data, be mapped to continuous scale either using an identity mapping or transformation, which for example could be useful if we want to map the value of a variable to the area of the symbol rather than its diameter.

Discrete scales work in a similar way. We can use `scale_colour_identity` and have in our data a variable with values that are valid colour names like "red" or "blue". However we can also assign the `colour` aesthetic to a factor with levels like "control", and "treatment", and these levels will be mapped to colours from the default palette, unless we chose a different one, or even use `scale_colour_manual` to assign whatever colour we want to each level to be mapped. The same is true for other discrete scales like `symbol`, `shape` and `linetype`. Be aware that for example for `colour`, and 'numbers' there are both discrete and continuous scales available.

Advanced scale manipulation requires the package `scales` to be loaded. Some simple examples follow.

```
fake2.data <- data.frame(
  y = c(rnorm(20, mean=20, sd=5), rnorm(20, mean=40, sd=10)),
  group = factor(c(rep("A", 20), rep("B", 20))),
  z = rnorm(40, mean=12, sd=6)
)
```

```
fig2 <-
  ggplot(data=fake2.data,
         aes(y=y, x=group, shape=group, colour=group, size=z)) +
  geom_point(alpha=0.3) + ylim(0, NA)
fig2
```



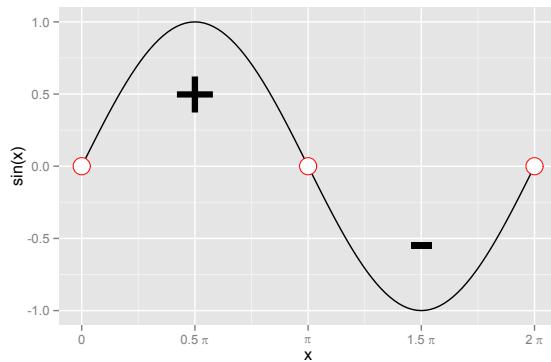
```
fig2 +
  scale_y_log10(breaks=c(10,20,30,40,50,60)) +
  stat_summary(fun.data = "mean_cl_normal",
               colour="black", size=1, alpha=1)

## Scale for 'y' is already present. Adding another scale for
## 'y', which will replace the existing scale.
## Error: Hmisc package required for this functionality.
Please install and try again.
```

## C.9 Adding annotations

Annotations use the data coordinates of the plot, but do not ‘inherit’ data or aesthetics from the ggplot.

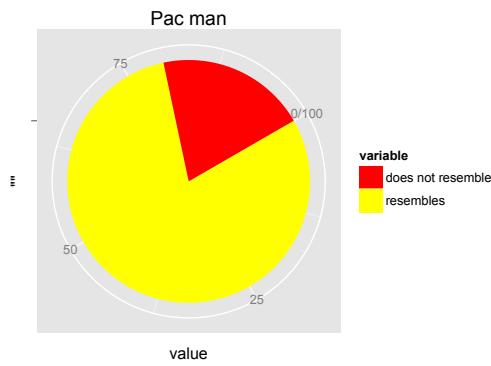
```
ggplot(data.frame(x=c(0, 2 * pi)), aes(x=x)) +
  stat_function(fun=sin) +
  scale_x_continuous(
    breaks=c(0, 0.5, 1, 1.5, 2) * pi,
    labels=c("0", expression(0.5~pi), expression(pi),
            expression(1.5~pi), expression(2~pi))) +
  labs(y="sin(x)") +
  annotate(geom="text",
          label=c("+", "-"),
          x=c(0.5, 1.5) * pi, y=c(0.5, -0.5),
          size=20) +
  annotate(geom="point",
          colour="red",
          shape=21,
          fill="white",
          x=c(0, 1, 2) * pi, y=0,
          size=6)
```



## C.10 Circular plots

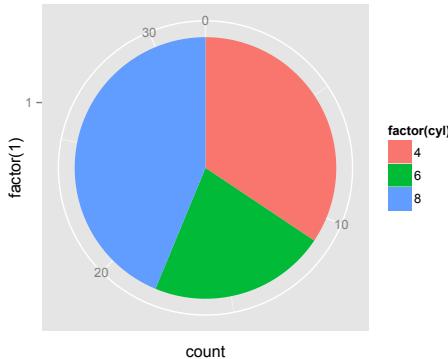
A funny example stolen from the `ggplot2` website at [http://docs.ggplot2.org/current/coord\\_polar.html](http://docs.ggplot2.org/current/coord_polar.html).

```
# Hadley's favourite pie chart
df <- data.frame(
  variable = c("resembles", "does not resemble"),
  value = c(80, 20)
)
ggplot(df, aes(x = "", y = value, fill = variable)) +
  geom_bar(width = 1, stat = "identity") +
  scale_fill_manual(values = c("red", "yellow")) +
  coord_polar("y", start = pi / 3) +
  labs(title = "Pac man")
```



Something just a bit more useful, also stolen from the same page:

```
# A pie chart = stacked bar chart + polar coordinates
pie <- ggplot(mtcars, aes(x = factor(1), fill = factor(cyl))) +
  geom_bar(width = 1)
pie + coord_polar(theta = "y")
```



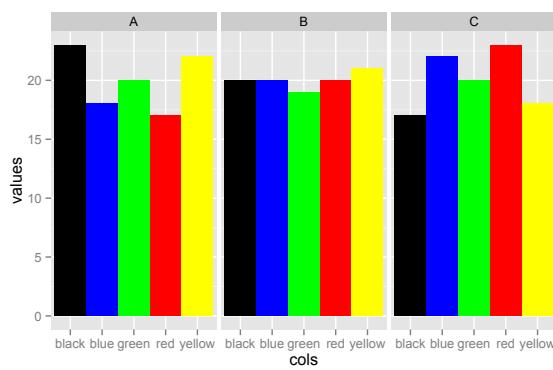
## C.11 Pie charts vs. bar plots example

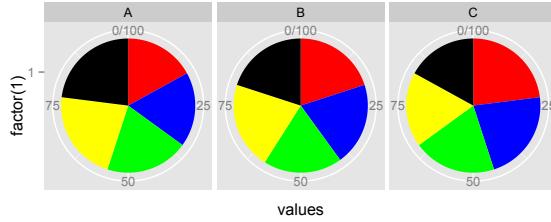
There is an example figure widely used in Wikipedia to show how much easier it is to ‘read’ bar plots than pie charts (<http://commons.wikimedia.org/wiki/File:Piecharts.svg?uselang=en-gb>).

Here is my `ggplot2` version of the same figure, using much simpler code and obtaining almost the same result.

```
example.data <-
  data.frame(values = c(17, 18, 20, 22, 23,
                       20, 20, 19, 21, 20,
                       23, 22, 20, 18, 17),
             examples= rep(c("A", "B", "C"), c(5,5,5)),
             cols = rep(c("red", "blue", "green", "yellow", "black"), 3)
  )

ggplot(example.data, aes(x=cols, y=values, fill=cols)) +
  geom_bar(width = 1, stat="identity") +
  facet_grid(.~examples) +
  scale_fill_identity()
ggplot(example.data, aes(x=factor(1), y=values, fill=cols)) +
  geom_bar(width = 1, stat="identity") +
  facet_grid(.~examples) +
  scale_fill_identity() +
  coord_polar(theta="y")
```





## C.12 A classical example about regression

This is another figure from Wikipedia <http://commons.wikimedia.org/wiki/File:Anscombe.svg?uselang=en-gb>. The original code (not run):

```
svg("anscombe.svg", width=10.5, height=7)
par(las=1)

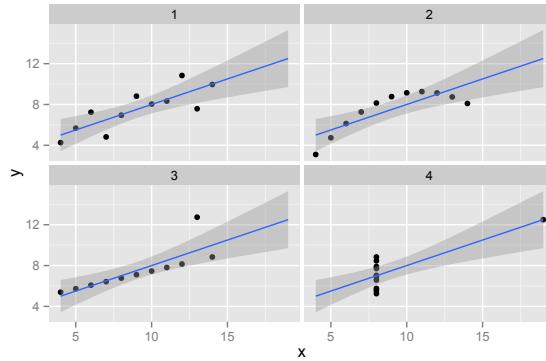
##-- some "magic" to do the 4 regressions in a loop:
ff <- y ~ x
for(i in 1:4) {
  ff[2:3] <- lapply(paste(c("y", "x"), i, sep=""), as.name)
  ## or   ff2 <- as.name(paste("y", i, sep=""))
  ##       ff3 <- as.name(paste("x", i, sep=""))
  assign(paste("lm.", i, sep=""), lmff, data= anscombe))
}

## Now, do what you should have done in the first place: PLOTS
op <- par(mfrow=c(2,2), mar=1.5+c(4,3.5,0,1), oma=c(0,0,0,0),
          lab=c(6,6,7), cex.lab=1.5, cex.axis=1.3, mgp=c(3,1,0))
for(i in 1:4) {
  ff[2:3] <- lapply(paste(c("y", "x"), i, sep=""), as.name)
  plot(ff, data =anscombe, col="red", pch=21, bg = "orange", cex = 2.5,
        xlim=c(3,19), ylim=c(3,13),
        xlab=eval(substitute(expression(x[i])), list(i=i)),
        ylab=eval(substitute(expression(y[i])), list(i=i)))
  abline(get(paste("lm.", i, sep=")), col="blue")
}

dev.off()
```

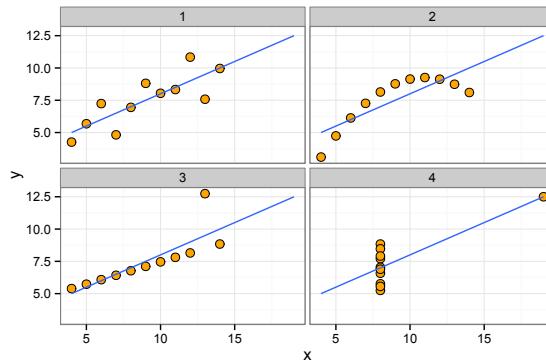
My version using ggplot2:

```
# we rearrange the data
my.mat <- matrix(as.matrix(anscombe), ncol=2)
my.anscombe <- data.frame(x = my.mat[, 1], y = my.mat[, 2], case=factor(rep(1:4, 10)))
# we draw the figure
ggplot(my.anscombe, aes(x,y)) +
  geom_point() +
  geom_smooth(method="lm") +
  facet_wrap(~case, ncol=2)
```



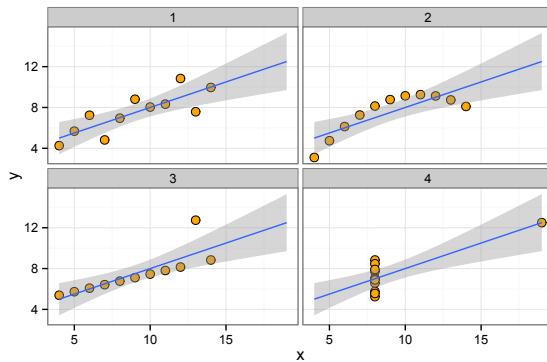
It is not much more difficult to make it look similar to the original

```
ggplot(my.anscombe, aes(x,y)) +
  geom_point(shape=21, fill="orange", size=3) +
  geom_smooth(method="lm", se=FALSE) +
  facet_wrap(~case, ncol=2) +
  theme_bw()
```



Although I think that the confidence bands make the point of the example much clearer

```
ggplot(my.anscombe, aes(x,y)) +
  geom_point(shape=21, fill="orange", size=3) +
  geom_smooth(method="lm") +
  facet_wrap(~case, ncol=2) +
  theme_bw()
```



This classical example from Anscombe [xxx](#) demonstrates four very different data sets that yield exactly the same results when a linear regression model is fit to them, including  $R^2 = 0.666$ . It is usually presented as a warning about the need to check model fits beyond looking at  $R^2$  and other parameter's estimates.

### C.13 Ternary plots

Being an extension to `ggplot2` the main difference is that a ternary plot can be created using `coord_tern` and that the three aesthetics `x`, `y`, `z` are required. By default the values of the variables mapped to these aesthetics are re-expressed as percentages or fractions. We present here only a few examples, and we encourage the readers to check the package's web site at <http://www.ggtern.com>.

For the first example we first generate some random data values from the uniform distribution:

```
# create some artificial data
my.trn1.data <- data.frame(x=runif(50), y=runif(50), z=runif(50))
```

A ternary plot is just a plot with a different system of coordinates, and can be obtained using `coord_tern`:

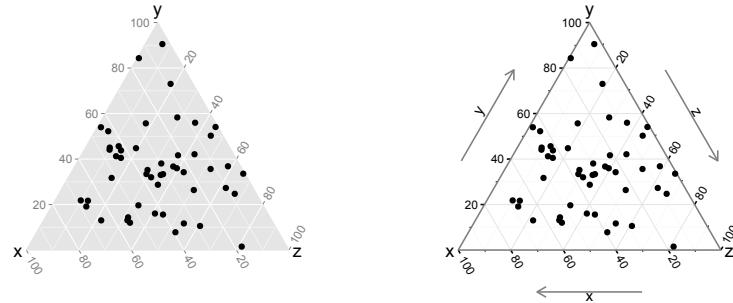
```
fig.trn <- ggplot(my.trn1.data, aes(x,y,z)) +
  coord_tern(L="x", T="y", R="z")
```

One can achieve a similar result by using `ggtern` instead of `ggplot`:

```
fig.trn <- ggtern(my.trn1.data, aes(x,y,z))
```

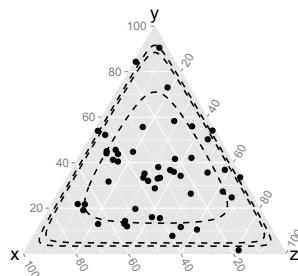
As with any other plot based on `ggplot2` one builds the plot by adding 'layers'. Themes are also supported.

```
fig.trn +
  geom_point()
fig.trn +
  geom_point() +
  theme_bw()
```



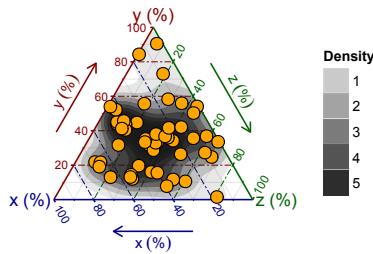
It is possible to also draw confidence regions:

```
fig.trn +
  geom_point() +
  geom_confidence()
```



Or density estimates. In this last version of the plot I adjust a few other aesthetics and refine the appearance of the plot:

```
fig.trn +
  stat_density2d(fullrange=T, n=200,
                 geom="polygon", fill="grey10",
                 aes(alpha =..level..)) +
  geom_point(shape=21, fill="orange", size=4) +
  labs(x="x (%)", y="y (%)", z="z (%)", alpha="Density") +
  theme_rgbw()
```



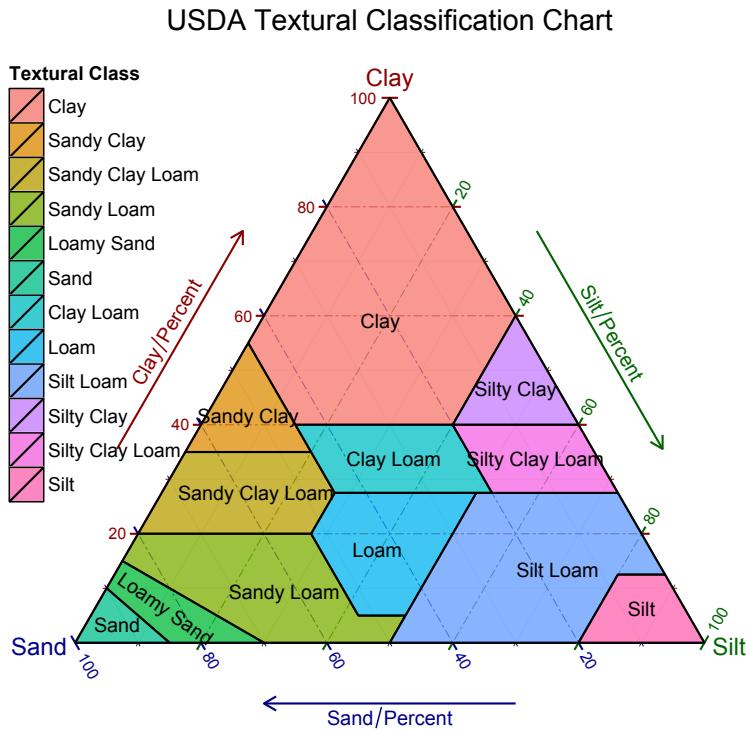
As a final example we reproduce an elaborate ternary plot from <http://www.ggtern.com/2014/01/15/usda-textural-soil-classification/>, the website of the package.

```
# Load the Data. (Available in ggtern 1.0.3.0 next version)
data(USDA)

# Put tile labels at the midpoint of each tile.
USDA.LAB = ddply(USDA, 'Label', function(df) {
  apply(df[, 1:3], 2, mean)
})

# Tweak
USDA.LAB$Angle = 0
USDA.LAB$Angle[which(USDA.LAB$Label == 'Loamy Sand')] = -35
```

```
# Construct the plot.
ggplot(data = USDA, aes(y=Clay, x=Sand, z=Silt,
                        color = Label,
                        fill = Label)) +
  coord_tern(L="x",T="y",R="z") +
  geom_polygon(alpha = 0.75, size = 0.5, color = 'black') +
  geom_text(data = USDA.LAB,
            aes(label = Label, angle = Angle),
            color = 'black',
            size = 3.5) +
  theme_rgbw() +
  theme_showsecondary() +
  theme_showarrows() +
  custom_percent("Percent") +
  theme(legend.justification = c(0, 1),
        legend.position      = c(0, 1),
        axis.tern.padding    = unit(0.15, 'npc')) +
  labs(title = 'USDA Textural Classification Chart',
       fill = 'Textural Class',
       color = 'Textural Class')
```



## C.14 Plotting data onto maps

Another extension to package `ggplot2` is package `ggmap`. Package `ggmap` makes it possible to plot data using normal `ggplot2` syntax on top of a map. Maps can be easily retrieved from the internet through different services. Some of these services require the user to register and obtain a key for access. As Google Maps do not require such a key for normal resolution maps, we use this service in the examples.

The first step is to fetch the desired map. One can fetch the maps base on any valid Google Maps search term, or by giving the coordinates at the center of the map. Although `zoom` defaults to "auto", frequently the best result is obtained by providing this argument. Valid values for `zoom` are integers in the range 1 to 20.

We will fetch maps from Google Maps. We have disabled the messages, to avoid repeated messages about Google's terms of use.

**Google Maps API Terms of Service:** <http://developers.google.com/maps/terms>

**Information from URL:** <http://maps.googleapis.com/maps/api/geocode/json?address=Europe&sensor=false>

**Map from URL:** <http://maps.googleapis.com/maps/api/staticmap?center=Europe&zoom=3&size=%20640x640&scale=%202&maptype=terrain&sensor=false>

We start by fetching and plotting a map of Europe of type `satellite`. We use the default extent `panel`, and also the extent `device` and `normal`. The `normal` plot includes axes showing the coordinates, while `device` does not show them, while `panel` shows axes but the map fits tightly into the drawing area:

```
Europe1 <- get_map("Europe", zoom=3, maptype="satellite")
ggmap(Europe1)

ggmap(Europe1, extent = "device")

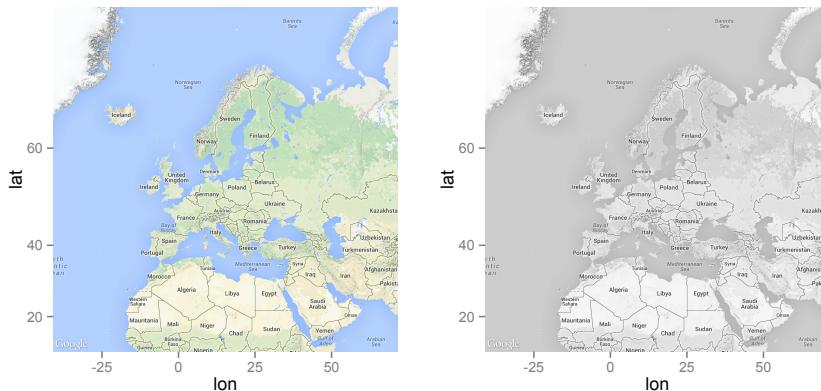
ggmap(Europe1, extent = "normal")
```



To demonstrate the option to fetch a map in black and white instead of the default colour version, we use a map of Europe of type `terrain`.

```
Europe2 <- get_map("Europe", zoom=3,
                    maptype="terrain")
ggmap(Europe2)

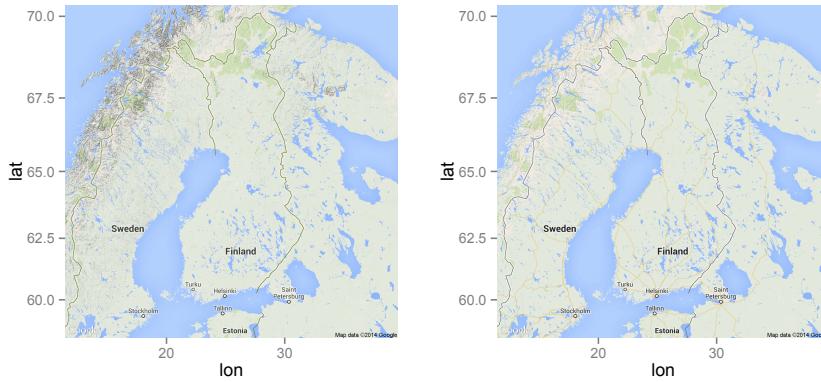
Europe3 <- get_map("Europe", zoom=3,
                    maptype="terrain",
                    color="bw")
ggmap(Europe3)
```



To demonstrate the difference between type `roadmap` and the default type `terrain`, we use the map of Finland. Note that we search for “Oulu” instead of “Finland” as Google Maps takes the position of the label “Finland” as the center of the map, and clips the northern part. By means of `zoom` we override the default automatic zooming onto the city of Oulu.

```
Finland1 <- get_map("Oulu", zoom=5, maptype="terrain")
ggmap(Finland1)

Finland2 <- get_map("Oulu", zoom=5, maptype="roadmap")
ggmap(Finland2)
```



We can even search for a street address, and in this case with high zoom value, we can see the building where one of us works:

```
BIO3 <- get_map("Viikinkaari 1, 00790 Helsinki",
                 zoom=18,
                 maptype="satellite")
ggmap(BIO3)
```



We will now show a simple example of plotting data on a map, first by explicitly giving the coordinates, and in the second example we show how to fetch from Google Maps coordinate values that can be then plotted. We use function `geocode`. In one example we use `geom_point` and `geom_text`, while in the second example we use `annotate`, but either approach could have been used for both plots:

```

viikki <- get_map("Viikki",
                   zoom=15,
                   maptype="satellite")

our_location <- data.frame(lat=c(60.225, 60.227),
                            lon=c(25.017, 25.018),
                            label=c("BIO3", "field"))

ggmap(viikki, extent = "normal") +
  geom_point(data=our_location, aes(y=lat, x=lon),
             size=4, colour="yellow") +
  geom_text(data=our_location, aes(y=lat, x=lon, label=label),
            hjust=-0.3, colour="yellow")

our_geocode <- geocode("Viikinkaari 1, 00790 Helsinki")
ggmap(viikki, extent = "normal") +
  annotate(geom="point",
          y=our_geocode[ 1, "lat"], x=our_geocode[ 1, "lon"],
          size=4, colour="yellow") +
  annotate(geom="text",
          y=our_geocode[ 1, "lat"], x=our_geocode[ 1, "lon"],
          label="BIO3", hjust=-0.3, colour="yellow")

```



Using `get_map` from package `ggmap` for drawing a world map is not possible at the time of writing. In addition a worked out example of how to plot shape files, and how to download them from a repository is suitable as our final example. We also show how to change the map projection. The example is adapted from a blog post at <http://rpsychologist.com/working-with-shapefiles-projections-and-world-maps-in-ggplot>.

We start by downloading the map data archive files from <http://www.naturalearthdata.com> which is available in different layers. We only use three of the available layers: ‘physical’ which describes the coastlines and a grid and bounding box, and ‘cultural’ which gives country borders. We save them in a folder with name ‘maps’, which is expected to already exist. After downloading each file, we unzip it.

```
oldwd <- setwd("./maps")

url_path <-
# "http://www.naturalearthdata.com/download/110m/"
  "http://www.naturalearthdata.com/http://www.naturalearthdata.com/download/110m/"

download.file(paste(url_path,
  "physical/ne_110m_land.zip",
  sep=""), "ne_110m_land.zip")
unzip("ne_110m_land.zip")

download.file(paste(url_path,
  "cultural/ne_110m_admin_0_countries.zip",
  sep=""), "ne_110m_admin_0_countries.zip")
unzip("ne_110m_admin_0_countries.zip")

download.file(paste(url_path,
  "physical/ne_110m_graticules_all.zip",
  sep=""), "ne_110m_graticules_all.zip")
unzip("ne_110m_graticules_all.zip")

setwd(oldwd)
```

We list the layers that we have downloaded.

```
ogrListLayers(dsn="./maps")
```

```
## Error: could not find function "ogrListLayers"
```

Next we read the layer for the coastline, and use `fortify` to convert it into a data frame. We also create a second version of the data using the Robinson projection.

```
wmap <- readOGR(dsn=".maps", layer="ne_110m_land")

## Error: could not find function "readOGR"

wmap.data <- fortify(wmap)

## Error: object 'wmap' not found

wmap_robin <- spTransform(wmap, CRS("+proj=robin"))

## Error: could not find function "spTransform"

wmap_robin.data <- fortify(wmap_robin)

## Error: object 'wmap_robin' not found
```

We do the same for country borders,

```
countries <- readOGR("./maps", layer="ne_110m_admin_0_countries")

## Error: could not find function "readOGR"

countries.data <- fortify(countries)

## Error: object 'countries' not found

countries_robin <- spTransform(countries, CRS("+init=ESRI:54030"))

## Error: could not find function "spTransform"

countries_robin.data <- fortify(countries_robin)

## Error: object 'countries_robin' not found
```

and for the graticule at 15° intervals, and the bounding box.

```
grat <- readOGR("./maps", layer="ne_110m_graticules_15")

## Error: could not find function "readOGR"

grat.data <- fortify(grat)

## Error: object 'grat' not found

grat_robin <- spTransform(grat, CRS("+proj=robin"))

## Error: could not find function "spTransform"

grat_robin.data <- fortify(grat_robin)

## Error: object 'grat_robin' not found

bbox <- readOGR("./maps", layer="ne_110m_wgs84_bounding_box")

## Error: could not find function "readOGR"
```

```

bbox.data <- fortify(bbox)

## Error: object 'bbox' not found

bbox_robin <- spTransform(bbox, CRS("+proj=robin"))

## Error: could not find function "spTransform"

bbox_robin.data <- fortify(bbox_robin)

## Error: object 'bbox_robin' not found

```

Now we plot the world map of the coastlines, on a longitude and latitude scale, as a `ggplot` using `geom_polygon`.

```

ggplot(wmap.data, aes(long,lat, group=group)) +
  geom_polygon() +
  labs(title="World map (longlat)") +
  coord_equal()

## Error: object 'wmap.data' not found

```

There is one noticeable problem in the map shown above: the Caspian sea is missing. We need to use aesthetic `fill` and a manual scale to correct this.

```

ggplot(wmap.data, aes(long,lat, group=group, fill=hole)) +
  geom_polygon() +
  labs(title="World map (longlat)") +
  scale_fill_manual(values=c("#262626", "#e6e8ed"),
                    guide="none") +
  coord_equal()

## Error: object 'wmap.data' not found

```

When plotting a map using a projection, many default elements of the `ggplot` theme need to be removed, as the data is no longer in units of degrees of latitude and longitude and axes and their labels are no longer meaningful.

```

theme_map_opts <-
  list(theme(panel.grid.minor = element_blank(),
            panel.grid.major = element_blank(),
            panel.background = element_blank(),
            plot.background = element_rect(fill="#e6e8ed"),
            panel.border = element_blank(),
            axis.line = element_blank(),
            axis.text.x = element_blank(),
            axis.text.y = element_blank(),
            axis.ticks = element_blank(),
            axis.title.x = element_blank(),
            axis.title.y = element_blank()))

```

Finally we plot all the layers using the Robinson projection. This is still a `ggplot` and consequently one can plot data on top of the map, being aware of the transformation of the scale needed to make the data location match locations in a map using a certain projection.

```

ggplot(bbox_robin.data, aes(long,lat, group=group)) +
  geom_polygon(fill="white") +
  geom_polygon(data=countries_robin.data,
               aes(long,lat, group=group,
                   fill=hole)) +
  geom_path(data=countries_robin.data,
            aes(long, lat, group=group, fill=NULL),
            linetype="dashed",
            color="grey50") +
  labs(title="World map (Robinson)") +
  coord_equal() +
  theme_map_opts +
  scale_fill_manual(values=c("black", "white"),
                    guide="none")

## Error: object 'bbox_robin.data' not found

```

## C.15 Inset plots using same data

Example from <http://stackoverflow.com/questions/20708012/embedding-a-subplot-in-ggplot-ggsubplot>, authored by Baptiste Auguié <http://baptiste.github.io/>.

```

d = data.frame(x = sort(rlnorm(300)),
                y = sort(rlnorm(300)),
                grp = 1)

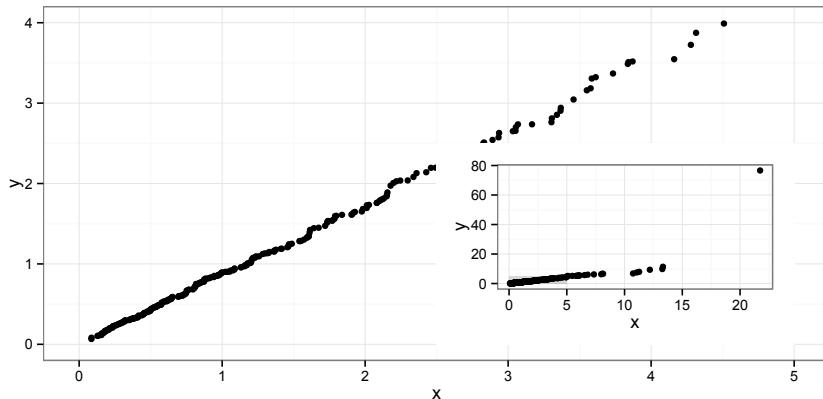
main <- ggplot(d, aes(x, y)) +
  geom_point() + theme_bw()

sub <- main +
  geom_rect(data=d[1,],
            xmin=0, ymin=0, xmax=5, ymax=5,
            fill="grey50", alpha=0.3)
sub$layers <- rev(sub$layers) # draw rect below

main +
  annotation_custom(ggplotGrob(sub),
                     xmin=2.5, xmax=5,
                     ymin=0, ymax=2.5) +
  scale_x_continuous(limits=c(0, 5)) +
  scale_y_continuous(limits=c(0, 4))

## Warning: Removed 25 rows containing missing values
(geom_point).

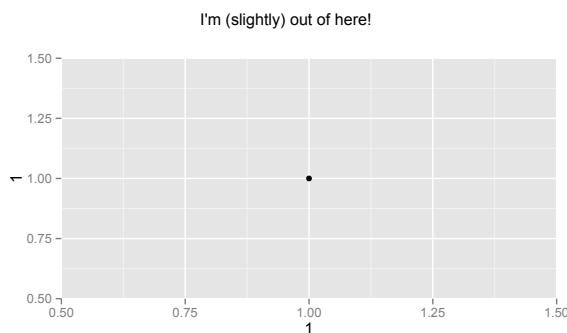
```



## C.16 Adding elements using grid

`ggplot2` creates the plots using package `grid`, consequently it is possible to manipulate `ggplot` objects using `grid` functions. Here we present a very simple example. For more information on using `grid` together with `ggplot2` please see [Murriel2009](#)

```
print(qplot(1, 1, vp=viewport(height=0.8))
grid.text(0.5, unit(1, "npc") - unit(1, "line"),
label="I'm (slightly) out of here!"))
```



## C.17 Generating output files

It is possible, when using RStudio, to directly export the displayed plot to a file. However, if the file will have to be generated again at a later time, or a series of plots need to be produced with consistent format, it is best to include the commands to export the plot in the script.

In R, files are created by printing to different devices. Printing is directed to a currently open device. Some devices produce screen output, others files. Devices depend on drivers. There are both devices that are part of R, and devices that can be added through packages.

A very simple example of PDF output (width and height in inches):

```
fig1 <- ggplot(data.frame(x=-3:3), aes(x=x)) +  
  stat_function(fun=dnorm)  
pdf(file="fig1.pdf", width=8, height=6)  
print(fig1)  
dev.off()
```

Encapsulated Postscript output (width and height in inches):

```
postscript(file="fig1.eps", width=8, height=6)  
print(fig1)  
dev.off()
```

There are Graphics devices for BMP, JPEG, PNG and TIFF format bitmap files. In this case the default units for width and height is pixels. For example we can generate TIFF output:

```
tiff(file="fig1.tiff", width=1000, height=800)  
print(fig1)  
dev.off()
```



## 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 3.0.3 (2014-03-06)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
##
## 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      stats     graphics  grDevices
## [5] utils     datasets  methods   base
```

```
##  
## other attached packages:  
## [1] scales_0.2.4  
## [2] microbenchmark_1.3-0  
## [3] ggtern_1.0.3.2  
## [4] ggmap_2.3  
## [5] photobiologygg_0.1.9  
## [6] plyr_1.8.1  
## [7] splus2R_1.2-0  
## [8] proto_0.3-10  
## [9] photobiologyAll_0.1.1  
## [10] photobiologySun_0.1.2  
## [11] photobiologyCry_0.1.2  
## [12] photobiologyPhy_0.2.5  
## [13] photobiologySensors_0.1.6  
## [14] photobiologyLEDs_0.1.1  
## [15] photobiologyLamps_0.1.10  
## [16] photobiologyFilters_0.1.8  
## [17] data.table_1.9.2  
## [18] photobiologyVIS_0.1.5  
## [19] photobiologyUV_0.2.8  
## [20] photobiology_0.3.2  
## [21] lubridate_1.3.3  
## [22] ggplot2_1.0.0  
## [23] knitr_1.6  
##  
## loaded via a namespace (and not attached):  
## [1] colorspace_1.2-4      digest_0.6.4  
## [3] evaluate_0.5.5       formatR_0.10  
## [5] gtable_0.1.2         highr_0.3  
## [7] labeling_0.2          lattice_0.20-27  
## [9] mapproj_1.2-2        maps_2.3-7  
## [11] MASS_7.3-29          memoise_0.2.1  
## [13] munsell_0.4.2        png_0.1-7  
## [15] Rcpp_0.11.2          reshape2_1.4  
## [17] RgoogleMaps_1.2.0.6  rjson_0.2.14  
## [19] RJSONIO_1.2-0.2       sp_1.0-15  
## [21] stringr_0.6.2         tools_3.0.3
```