Introduction to casper

Jose Eduardo Meireles

2016-11-08

The goal of `casper` is first and foremost to provide a `spectra` class for `R` that exposes a standard interface and patafrom that allows other `R` packages to build on. The package will provide very basic IO, plotting and conversion functionality, but that is about it. `casper` is implemented with ease of use in mind, but shouldn't slow you down.

Installing and loading `casper`

The best way to get `casper` is to install it directly from the *github repository*. You will need the `devtools` package to do it though.

```
library("devtools")
install_github("meireles/casper")
```

Assuming that everything went smoothly, you should be able to load `casper` like any other package.

```
library("casper")
```

Reading spectra and creating a `spectra` object

First, explore the example dataset `spec_example`

As already stated, `casper` comes with limited IO capabilities. To illustrate how to create a `spectra` object, we will use an example dataset called `spec_example` which is in `matrix` format. Samples are in rows, and wavelengths in columns, and the first column is the sample name (in this case, a species name). The column names match wavelength labels. I tried to format `spec_example` to mimic the is typical result of a `read.csv` command.

```
# Example spectral dataset in matrix format.
spec_example[1:4, 1:3]
```

```
##      species     400                 401
## [1,] "species_7" "0.0410280788726612" "0.041068460214908"
## [2,] "species_6" "0.0410014027444064" "0.04104068877155"
## [3,] "species_6" "0.0410053662963379" "0.0410446038853763"
## [4,] "species_7" "0.0409941662890207" "0.0410332454133088"
```

```
# Note that this is NOT a spectra object.
# You can verify this by asking what class `spec_example` is.
class(spec_example)
```

```
## [1] "matrix"
```

```
# An alternative is to use casper's `is_spectra()` function.
is_spectra(spec_example)
```

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

Constructing a `spectra` object

The `spectra` class holds the essential information used in spectral dataset: reflectance, wavelengths, etc. The class has a bunch of requirements in terms of both format and values, for instance, relative reflectance must be between 0 and 1.

If your data is in a matrix with the same format as `spec_example` (check above for details), you can construct a `spectra` object by calling the `as.spectra()` function.

```
# Make a spectra object if you have a matrix in the right format
spec = casper::as.spectra(spec_example)

# Did it work?
is_spectra(spec)
```

```
## [1] TRUE
```

Alternatively, you can create a `spectra` object using the more flexible `spectra()` constructor, which takes three arguments: (1) a reflectance matrix, (2) the wavelength numbers and (3) the sample names.

```
# (1) Create a reflectance matrix.
#     In this case, by removing the species column
rf = spec_example[ , -1 ]

# Check the result
rf[1:4, 1:3]
```

```
##      400                 401                 402
## [1,] "0.0410280788726612" "0.041068460214908"  "0.0410958153498105"
## [2,] "0.0410014027444064" "0.04104068877155"   "0.0410669861589336"
## [3,] "0.0410053662963379" "0.0410446038853763" "0.0410708238395667"
## [4,] "0.0409941662890207" "0.0410332454133088" "0.0410593605341906"
```

```
# (2) Create a vector with wavelength labels that match
#     the reflectance matrix columns.
wl = colnames(rf)

# Check the result
wl[1:6]
```

```
## [1] "400" "401" "402" "403" "404" "405"
```

```
# (3) Create a vector with sample labels that match
#     the reflectance matrix rows.
#     In this case, use the first colum of spec_example
sn = spec_example[ , 1]

# Check the result
sn[1:6]
```

```
## [1] "species_7" "species_6" "species_6" "species_7" "species_7" "species_9"
```

```
# Finally, construct the spectra object using the `spectra` constructor
spec = spectra(reflectance = rf, wavelengths = wl, sample_names = sn)

# And hopefully this worked fine
is_spectra(spec)
```

```
## [1] TRUE
```

Converting a spectra object into a matrix

It is possible to convert a `spectra` object to a matrix format, using the `as.matrix()` function. `casper` will (1) place wavelength in columns, assigning wavelength labels to `colnames`, and (2) samples in rows, assigning sample names to `rownames`. Since `R` imposes strict on column and row name formats (e.g. no duplicates), `as.matrix()` tries to fix potential dimname issues by default (see the argument `fix_dimnames`).

```
# Make a matrix from a `spectra` object
spec_as_mat = as.matrix(spec, fix_dimnames = TRUE)
```

```
## Error in as.matrix(spec, fix_dimnames = TRUE): unused argument (fix_dimnames = TRUE)
```

```
spec_as_mat[1:4, 1:3]
```

```
## Error in eval(expr, envir, enclos): object 'spec_as_mat' not found
```

Exploring `spectra` object

`casper` exposes a few ways to plot and query spectral data in `spectra` format.

Plotting

The workhorse function for plotting `spectra` is `plot()`. It will jointly plot each spectrum in the `spectra` object. You should be able to pass the usual plot arguments to it, such as `col`, `ylab`, etc.

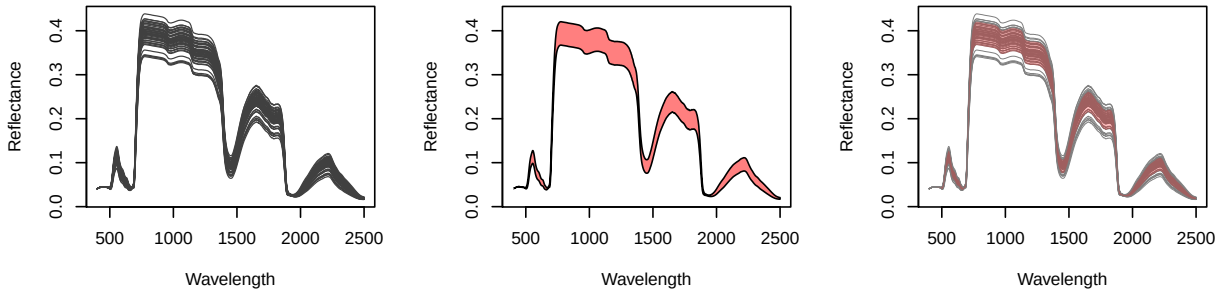
You can also plot the quantile of a `spectra` object with `plot_quantile()`. It's second argument, `total_prob`, is the total "mass" that the quantile encompasses. For instance, a `total_prob = 0.95` covers 95% of the variation in the `spectra` object; i.e. it is the `0.025 to 0.975` quantile. The quantile plot can stand alone or be added to a current plot if `add = TRUE`.

```
par(mfrow = c(1, 3))

# Simple spectra plot
plot(spec, lwd = 0.75, lty = 1, col = "grey25")

# Stand along quantile plot
plot_quantile(spec, total_prob = 0.8,
              col = rgb(1, 0, 0, 0.5), border = TRUE)

# Combined quantile and individual spctra plot
plot(spec, lwd = 0.25, lty = 1, col = "grey50")
plot_quantile(spec, total_prob = 0.8,
              col = rgb(1, 0, 0, 0.25), add = TRUE, border = FALSE)
```



Querying

`casper` lets you query the `spectra` object and get summary infomation. You can easly get sample names with `sample_names()` and wavelength labels with `wavelengths()`. It is also possible to recover the

```
# Get the vector of all sample names
# Note that duplicate sample names are permitted
n = sample_names(spec)
n[1:5]
```

```
## [1] "species_7" "species_6" "species_6" "species_7" "species_7"
```

```
# Or get the vector of wavelengths
w = wavelengths(spec)
w[1:5]
```

```
## [1] "400" "401" "402" "403" "404"
```

```
# You can also get the dimensions of your `spectra` object
dim(spec)
```

```
##     n_samples n_wavelengths
##            50          2101
```

Subsetting spectra

You can subset the `spectra` using a notation *similar* to the `[ i , j]` function used in matrices and data.frames. The first argument in `[ i, ]` matches *sample names*, whereas the second argument `[ , j ]` matches the *wavelength names*. Here are some important differences between how `[` works in matrices and in `specrta`:

- `x[ 1:3 , ]` will keep the first three samples of `x`.
- `x[ "sp_1" , ]` keeps **all** entries in `x` where sample names match `"sp_1"`
- `x[  , 800:900 ]` will keep wavelengths between 800 and 900.
- `x[  , 1:5 ]` will **fail**!. wavelengths cannot be subset by index!

```
# Subset spectra to all entries where sample_name matches "species_8"
spec_sp8 = spec[ "species_8", ]

# And maybe further subset to the visible wavelengths only
spec_sp8 = spec_sp8[ , 400:700 ]

dim(spec_sp8)
```

```
##     n_samples n_wavelengths
##             5           301
```

```
# Note that you can subset by wavelength using numerics or characters.
reflectance(spec_sp8[ 1 , "405"]) == reflectance(spec_sp8[ 1 , 405])
```

```
##      [,1]
## [1,] TRUE
```

```
# But you CANNOT use indexes to subset wavelengths!
# Something that is obvioulsy an index will fail. For instance, using 2 instead of 401
spec_sp8[ , 2 ]
```

```
## Error in `[.spectra`(spec_sp8, , 2): Wavelength subscript out of bounds. Use wavelength labels instea
```

```
# However, if you use 2000:2001 you will NOT get the two last bands, but instead
# wavelengths "2000" and "2001".Bottomline, be careful not to use indexes!
```

Manipulating samples and wavelength labels

```
#x1 = spec[ "species_8", ]
#plot(spec[ "species_8", ], lwd = 1, lty = 1, col = "red4", add = TRUE)
#dim(x1)
```

Updating sample names or wavelength labels