CWRU DSCI351-351M-453: Week5a-HyperSpec Package Review(CWRU, Pitt, UCF, UTRGV)

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27 September, 2022

Contents

5.1.2.1   Class Readings, Assignments, Syllabus Topics

5.1.2.1.1 Reading, Lab Exercises, SemProjects

- Readings:
  - For today: OIS5, EDA32058
  - For next class: R4DS4-6
- Laboratory Exercises:
  - LE3 : Has been given out
  - **LE3 : Is due Thursday October 6th**
- Office Hours: (Class Canvas Calendar for Zoom Link)
  - Wednesday @ 4:00 PM to 5:00 PM, Will Oltjen
  - Saturday @ 3:00 PM to 4:00 PM, Kristen Hernandez
  - **Office Hours are on Zoom, and recorded**
- Semester Projects
  - DSCI 451 Students Biweekly Update 1 Due
  - DSCI 451 Students
    * Next **Report Out #1 is Due Friday September 30th**
  - All DSCI 351/351M/451 Students:
    * **Peer Grading of Report Out #1 is Due October 11th, 2022**
  - Exams
    * MidTerm: Tuesday October 18th, in class or remote, 11:30 - 12:45 PM
    * Final: Monday December 19, 2022, 12:00PM - 3:00PM, Nord 356 or remote

5.1.2.2 Textbooks

- Peng: R Programming for Data Science
- Peng: Exploratory Data Analysis with R
- Open Intro Stats, v4
- Wickham: R for Data Science
- Hastie: Intro to Statistical Learning with R, 2nd Ed.

Introduction to R and Data Science

- For R, Coding, Inferential Statistics
  - Peng: R Programming for Data Science
  - Peng: Exploratory Data Analysis with R

Textbooks for this class

- OIS = Diez, Barr, Çetinkaya-Runde: Open Intro Stat v4
- R4DS = Wickham, Grolemund: R for Data Science

Textbooks for DSCI353/353M/453, And in your Repo now

- ISLR = James, Witten, Hastie, Tibshirani: Intro to Statistical Learning with R 2nd Ed.
- ESL = Trevor Hastie, Tibshirani, Friedman: Elements of Statistical Learning
- DLwR = Chollet, Allaire: Deep Learning with R

Magazine Articles about Deep Learning

- DL1 to DL12 are "Deep Learning" articles in 3-readings/2-articles/

5.1.2.2.1 Tidyverse Cheatsheets, Functions and Reading Your Code

- Look at the Tidyverse Cheatsheet

  - **Tidyverse For Beginners Cheatsheet**
    * In the Git/20s-dsci353-353m-453-prof/3-readings/3-CheatSheets/ folder
  - **Data Wrangling with dplyr and tidyr Cheatsheet**

  Tidyverse Functions & Conventions

- The pipe operator `%>%`
- Use `dplyr::filter()` to subset data row-wise.
- Use `dplyr::arrange()` to sort the observations in a data frame
- Use `dplyr::mutate()` to update or create new columns of a data frame
- Use `dplyr::summarize()` to turn many observations into a single data point
- Use `dplyr::arrange()` to change the ordering of the rows of a data frame
- Use `dplyr::select()` to choose variables from a tibble,
    * keeps only variables you mention
- Use `dplyr::rename()` keeps all the variables and renames variables
    * rename(iris, petal_length = Petal.Length)
- These can be combined using `dplyr::group_by()`
    * which lets you perform operations "by group".
- The `%in%` matches conditions provided by a vector using the c() function
- The **forcats** package has tidyverse functions
    * for factors (categorical variables)
- The **readr** package has tidyverse functions
    * to read_..., melt_... col_..., parse_... data and objects

Reading Your Code: Whenever you see

- The assignment operator `<-`, think **"gets"**
- The pipe operator, `%>%`, think **"then"**

5.1.2.2.2 Syllabus

5.1.2.3 Background

5.1.2.3.1 Spectra - What are they?

- "a specific set of values that can vary infinitely within a continuum"
- Generally: 2-dimensional (sometimes higher) dimensional data,
    - where the first dimension identifies points along a continuum,
    - and the second dimension the values of a response of interest
    - at the corresponding points
- Examples: Optical, Mass, Political Alignment

5.1.2.3.2 Spectral Data - How do we store them?

- Proprietary file format: not so useful
- .csv files (ASCII): better ~ excel, R
- .spc files (Binary): good ~ R

5.1.2.3.3 hyperSpec - How to manipulate .spc files in R

- http://hyperspec.r-forge.r-project.org/
- Handles spectral data
- Features:
    - Convenient import,
    - spectral range selection,
    - shifting,

    - plotting/viewing,
    - normalization,
    - smoothing,
    - correction,
    - arithmetic,

Day:Date	Foundation	Practicum	Reading	Due
w01a:Tu:8/30/22	ODS Tool Chain	R, Rstudio, Git		
w01b:Th:9/1/22	Setup ODS Tool Chain	Bash, Git, Slack, Agile	PRP4-33	LE1
w02a:Tu:9/6/22	Bash-Git-Knuth-Lit.Prog.	RIntroR	PRP35-64	
w02b:Th:9/8/22	What is Data Science	OIS:Intro2R	OIS1,2	
w02Pr:Fr:9/9/22			PRP65-93	451 Update1
w03a:Tu:9/13/22	Data Intro	Data Analytic Style	PRP94-116	LE2 **LE1 Due**
w03b:Th:9/15/22	Rand. Var. Normal Dist.	Git, Rmds, Loops	OIS4	
w04a:Tu:9/20/22	Tidy Check Explore	Tidy GapMinder	EDA1-31	
w04b:Th:9/22/22	Inference, DSCI Process	Other Distrib. 7 ways	R4DS1-3	LE3 **LE2 Due**
w04Pr:Fr:9/23/22			EDA32-58	451 Update2
w05a:Tu:9/27/22	OIS4 Rand. Var.	EDA of PET Degr.	OIS5	
w05b:Th:9/29/22	OIS5 Found. of Infer.	Multivar Corr. Plot	R4DS4-6	
w05Pr:Fr:9/30/22				451 RepOut1
w06a:Tu:10/4/22	Pred., Algorithm, Model	Anscombe's Quartets	R4DS7-8	
w06b:Th:10/6/22	EDA stats, vis	Summ. Stats & Vis.	R4DS9-16	LE4 **LE3 Due**
w06Pr:Fr:10/7/22	Corr. Coeff. Pairs Plots			451 Update3
w07a:Tu:10/11/22	Confidence Intervals	Penguins	OIS6.1-2	**PeerRv1 Due**
w07b:Th:10/13/22	Midterm Rev.	Hypo.Test, Sampl. Dist.		
w08a:Tu:10/18/22	**MIDTERM**	**EXAM**		
w08b:Th:10/20/22	Programming & Coding	Coding Expect.		**LE4 Due**
w08Pr:Fr:10/21/22				451 Update4
Tu:10/24,25	**CWRU**	**FALL BREAK**	R4DS17-21	
w09b:Th:10/27/22	Cat. Inf. 1 & 2 propor.	Indep. Test,2-way tables	OIS6.3-4	LE5
w09Pr:Fr:10/28/22				451 RepOut2
w10a:Tu:11/1/22	Goodness of Fit, χ^2 test	t-tests 1&2 means	OIS7.1-4	
w10b:Th:11/3/22	Num. Infer, Cont. Tables	Stat. Power		
w10Pr:Fr:11/4/22				451 Update5
w11a:Tu:11/8/22	Sample & Effect Size	Stat. Power GGmap	OIS8	**PeerRv2 Due**
w11b:Th:11/10/22	Inf. 4 Regr, Test & Train	Curse of Dimen.	ISLR1,2.1,2	LE6 **LE5 Due**
w12a:Tu:11/15/22	Lin. Regr. Part 1	Residuals	OIS9	
w12b:Th:11/17/22	Lin. Regr. Part 2	Regr. Diagnostics		
w12Pr:Fr:11/18/22				451 Update6
w13a:Tu:11/22/22	Mult. Lin. Regr.	Var. & Mod. Selec.,	ISLR3.1	LE7 **LE6 due**
w13b:Th:11/24/22	Log. Regr.	GIS Trends	ISLR3.2	
w13Pr:Fr:11/25/22				451 RepOut3
w14a:Tu:11/23/22	Classificat., Sup. Lrning	Caret, Broom 4 modeling	ISLR4.1-3	
Th,Fr:11/24,25	**THANKSGIVIING**	**Vacation**		
w15a:Tu:11/29/22		Clustering		**PeerRv3 Due**
w15b:Th:12/1/22	Big Data Analytics	Dist. Comp., Hadoop		
w15SPr:Fr:12/2/22		Read Article by	Mirletz,2015	
w16a:Tu:12/6/22	Final Exam Review			
w15b:Th:12/8/22				LE7 due
Friday 12/12	**SemProj**	**Final Report**		**SemProj4 due**
Monday 12/19	**FINAL EXAM**	**12:00-3:00pm**	Nord 356	or remote

Figure 1: DSCI351-351M-451 Syllabus

- initial data analysis

5.1.2.4 hyperSpec Examples

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union

## Loading required package: lattice

## Loading required package: grid

## Loading required package: ggplot2

## Loading required package: xml2

## Package hyperSpec, version 0.100.0
##
## To get started, try
##    vignette ("hyperspec")
##    package?hyperSpec
##    vignette (package = "hyperSpec")
##
## If you use this package please cite it appropriately.
##    citation("hyperSpec")
## will give you the correct reference.
##
## The project homepage is http://hyperspec.r-forge.r-project.org

##
## Attaching package: 'hyperSpec'

## The following object is masked from 'package:dplyr':
##
##     collapse
```

5.1.2.4.1 File Import   Can import spectra

- As .csv files
- Or as binary .spc files

```
# Read one .spc file and check its structure
# Use relative file paths
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_00_ex320.spc"
step0 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
class(step0)
```

```
## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"
```

```
step0
```

```
## hyperSpec object
##    1 spectra
##    4 data columns
##    301 data points / spectrum
## wavelength: lambda/nm [numeric] 330.00 331.07 ... 630
## data:  (1 rows x 4 columns)
##    1. z: x/"a. u." [numeric] 0
##    2. z.end: x/"a. u." [numeric] 0
##    3. spc: I/"a. u." [matrix, array301] 95.5881 98.6830 ... 94.45682
##    4. filename: filename [character] ./data/pet_unstab_cyclic_quv/sa19603_00_ex320.spc
```

```
# Plot with hyperSpec base plotting
```

```
plotspc(step0)
```

5.1.2.4.2 Basic Plotting
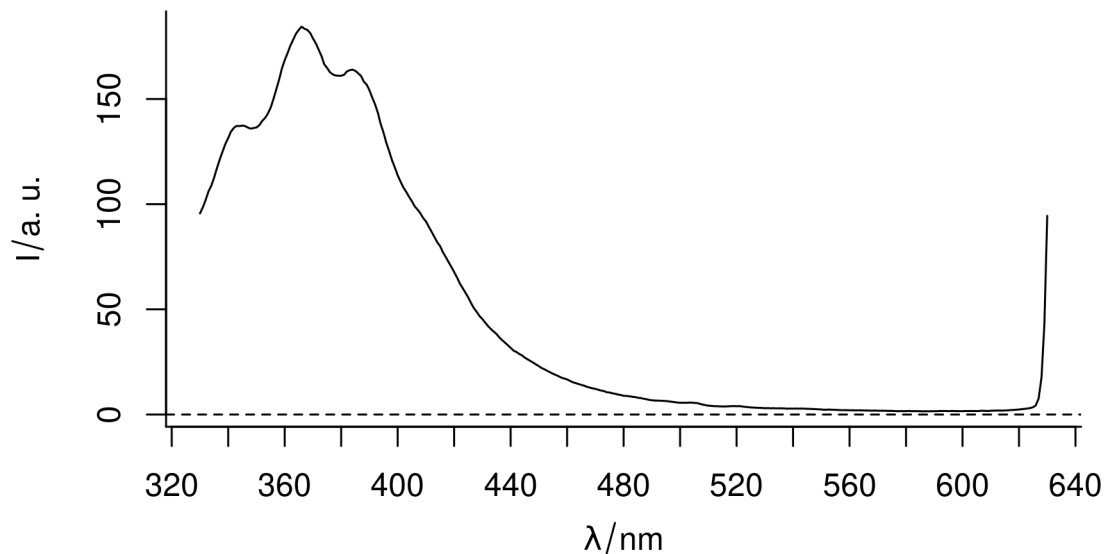
5.1.2.4.3 Multiple .spc Files?

- (Purposefully without a loop, apply command or pipes)

```
# Read multiple .spc files
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_00_ex320.spc"
step0 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_22_ex320.spc"
step1 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_23_ex320.spc"
step2 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_24_ex320.spc"
step3 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_25_ex320.spc"
step4 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_26_ex320.spc"
step5 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_27_ex320.spc"
step6 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
curfile <- "./data/pet_unstab_cyclic_quv/sa19603_28_ex320.spc"
step7 <- read.spc(curfile)
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 38 > 1' in coercion
## to 'logical(1)'
```

```
# Use Collapse to combine spectra
```

```
spec <- hyperSpec::collapse(step0, step1, step2, step3, step4, step5,
                            step6, step7)
class(spec)
```

5.1.2.4.4 Combine into one object (Good News!)

```
## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"
spec
```

```
## hyperSpec object
##    8 spectra
##    4 data columns
##    301 data points / spectrum
## wavelength: lambda/nm [numeric] 330.00 331.07 ... 630
## data:  (8 rows x 4 columns)
##    1. z: x/"a. u." [numeric] 0 0 ... 0
##    2. z.end: x/"a. u." [numeric] 0 0 ... 0
```

```
##     3. spc: I/"a. u." [AsIs matrix x 301] 95.58810 18.86919 ... 1000
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/sa19603_00_ex320.spc ./data/pet_uns
```

```
plotspc(spec)
```

5.1.2.4.5 Basic Plotting
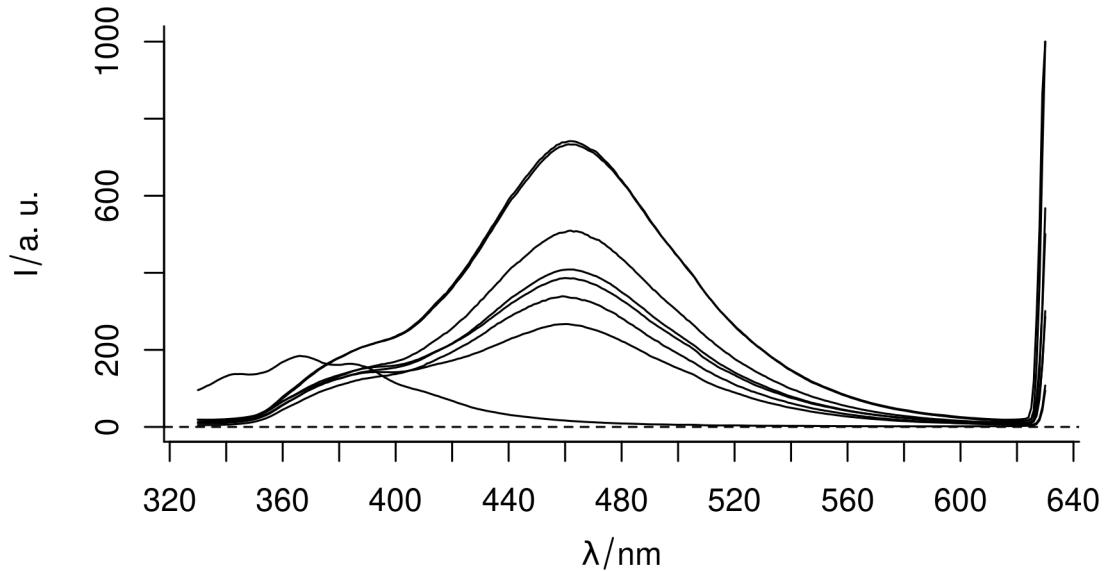

```
# Subset and redefine the hyperSpec object according to wavelength
```

```
spec <- spec[,, min ~ 600]
spec
```

5.1.2.4.6 Spectral Range Selection

```
## hyperSpec object
##     8 spectra
##     4 data columns
##     271 data points / spectrum
## wavelength: lambda/nm [numeric] 330.00 331.07 ... 600
## data:   (8 rows x 4 columns)
##     1. z: x/"a. u." [numeric] 0 0 ... 0
##     2. z.end: x/"a. u." [numeric] 0 0 ... 0
##     3. spc: I/"a. u." [AsIs matrix x 271] 95.58810 18.86919 ... 25.40894
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/sa19603_00_ex320.spc ./data/pet_uns
```

```
plotspc(spec)
```

5.1.2.4.7 Basic Plotting
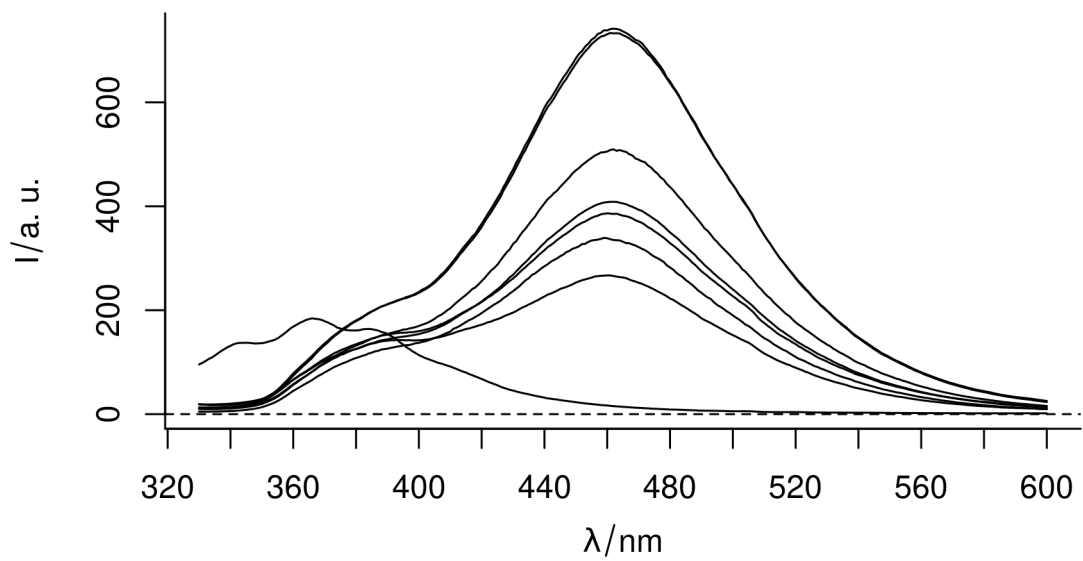
```
# Perform spectral subtraction

sub <- step7 - step0
plotspc(sub[,, min ~ 600])
```

5.1.2.4.8 Spectral Arithmetic (Subtraction)
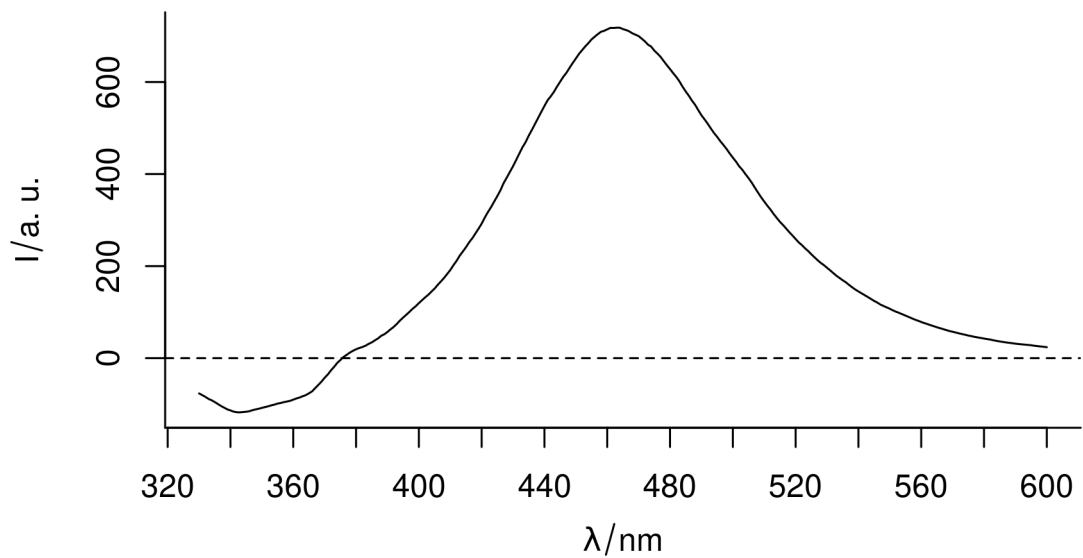

```
# Let's look at some fake IR data
ir.spc <- chondro
ir.spc
```

5.1.2.4.9 Removing Bad Data

```
## hyperSpec object
##     875 spectra
##     5 data columns
##     300 data points / spectrum
```

```
## wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
## data:   (875 rows x 5 columns)
##    1. y: y [numeric] -4.77 -4.77 ... 19.23
##    2. x: x [numeric] -11.55 -10.55 ... 22.45
##    3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
##    4. clusters: clusters [factor] matrix matrix ... lacuna + NA
##    5. spc: I / a.u. [matrix, array300] 501.8194 500.4552 ... 169.2942
```

```
plotspc(ir.spc, spc.nmax = length(ir.spc))
```
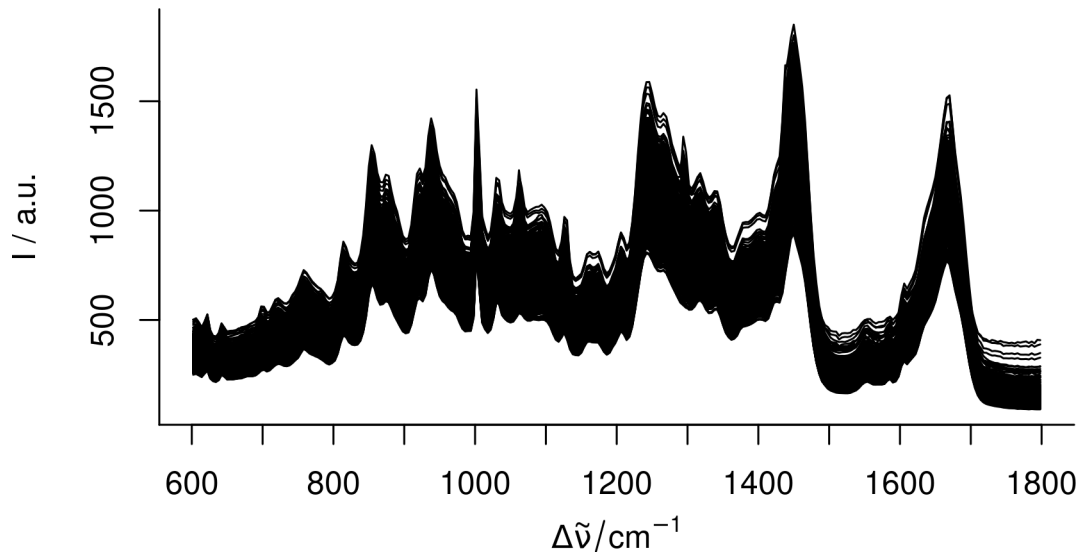


```
# Define any point above 1500 as bad
high.int <- apply(ir.spc > 1500, 1, any)

# Maximum should at least be 0.1
low.int <- apply(ir.spc, 1, max) < 0.1

# Apply Conditions
ir.spc <- ir.spc[!high.int & !low.int]
```

5.1.2.4.10 Removing Bad Data

```
plotspc(ir.spc, spc.nmax = length(ir.spc))
```

5.1.2.4.11 Removed the bad spectra
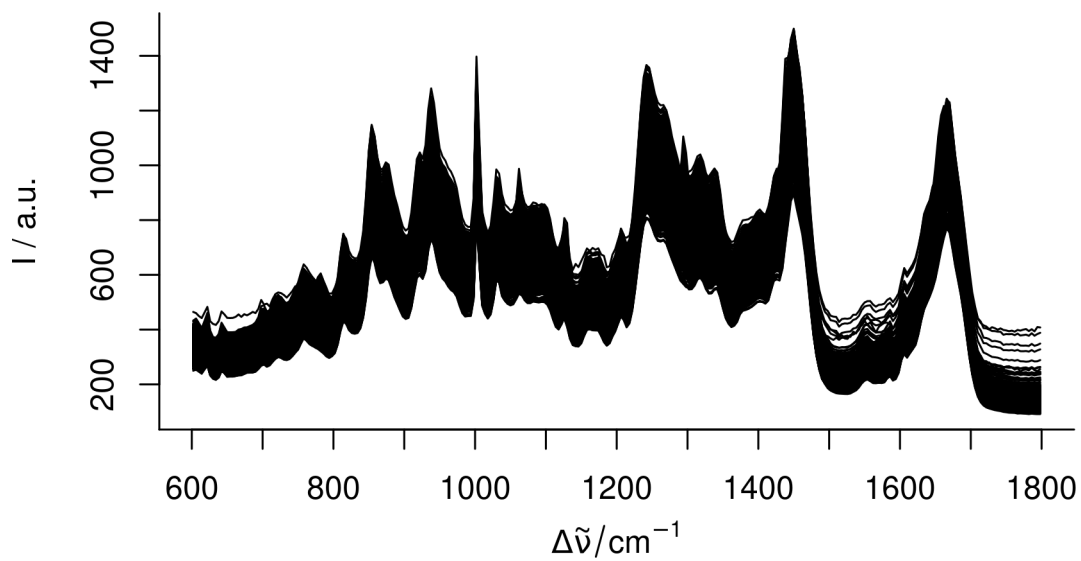
```
# Apply baseline correction function
blcorr <- spc.fit.poly.below(ir.spc)

# Subtract away correction from original
ir.spc <- ir.spc - blcorr
```

5.1.2.4.12   cq.abs.step0 Correction (One of many options)

```
plotspc(ir.spc)
```

5.1.2.4.13   Corrected Spectra!
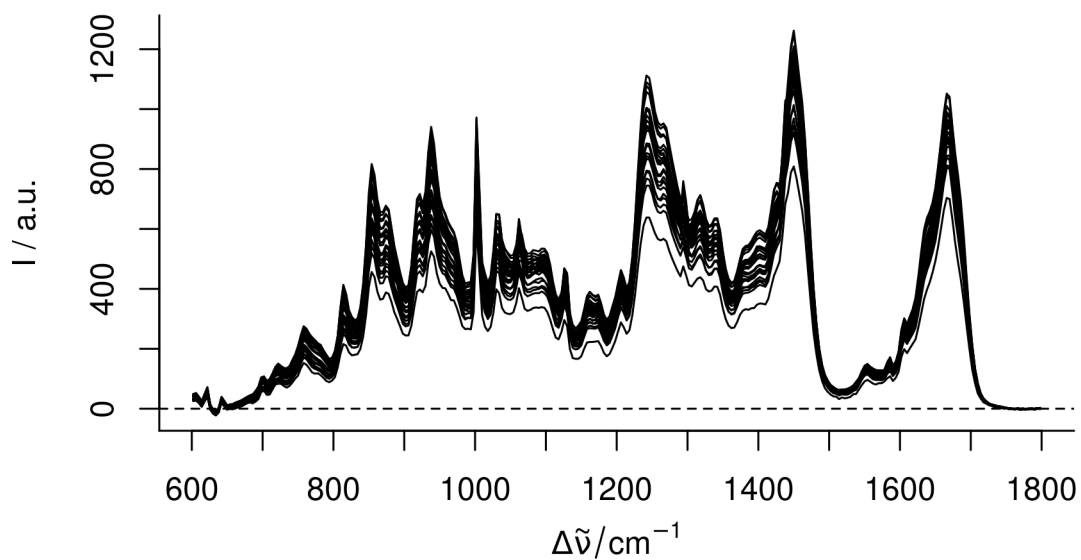
5.1.2.5   Example of using "Key Files" for sample Metadata

```
## Read keyfile(s) and set classes

pet.key <-
  read.csv("./data/pet_unstab_cyclic_quv/3m_sample_key.csv")
pet.key$Sample <- as.character(pet.key$Sample)
pet.key$Product <- as.character(pet.key$Product)
pet.key$Exposure <- as.character(pet.key$Exposure)
pet.key$Step_Retained <- as.character(pet.key$Step_Retained)

## Read step 0 (Unexposed) CyclicQUV Optical Absorbance Data

filenames <-
  list.files(path = "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/",
             pattern = "\\.spc$")

# Read Files, Here using lapply

cq.abs.step0 <- lapply(filenames, function(i) {
  read.spc(paste(
    "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/",
    i,
    sep = ""
  ))
})
```

5.1.2.5.1 Load Cyclic QUV Absorbance Data Set

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3213 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3215 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3763 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3215 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3215 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3215 > 1' in
## coercion to 'logical(1)'
```
```
# Combine resulting list into one hyperSpec object

cq.abs.step0 <-
  hyperSpec::collapse(cq.abs.step0[1:length(cq.abs.step0)])

# Add step data

cq.abs.step0@data$step <- 0


## Extract sample number from file name using sub (grep)
```

```r
## to pull the sample number from the file name
## match to row in the keyfile

cq.abs.step0@data$sample <- filenames %>%
  sub(pattern = "-es00-ms00-mn01_uvvs01.spc", replacement = "") %>%
  sub(pattern = "_", replacement = ".")

# Match material info from key file and add to hyperSpec object

rows <- cq.abs.step0@data$sample %>% pmatch(pet.key[, 1])
cq.abs.step0@data$material <- pet.key[rows, 2]

## Read step 1 CyclicQUV Optical Absorbance Data

filenames <-
  list.files(path = "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step1/",
             pattern = "\\.SPC$")

# Read Files

cq.abs.step1  <- lapply(filenames, function(i) {
  read.spc(paste(
    "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step1/",
    i,
    sep = ""
  ))
})
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'

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## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
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## to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'
```

```
## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
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## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
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## to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 57 > 1' in coercion
## to 'logical(1)'
```

```r
# Combine resulting list into one hyperSpec object

cq.abs.step1 <-
  hyperSpec::collapse(cq.abs.step1[1:length(cq.abs.step1)])

# Add step data

cq.abs.step1@data$step <- 1


## Extract sample number from file name using sub (grep)
## to pull the sample number from the file name match to row in the keyfile

cq.abs.step1@data$sample <- filenames %>%
  sub(pattern = "-es01-ms01-mn01_uvvs01.SPC", replacement = "") %>%
  sub(pattern = "_", replacement = ".")

# Match material info from key file and add to hyperSpec object

rows <- cq.abs.step1@data$sample %>% pmatch(pet.key[, 1])
cq.abs.step1@data$material <- pet.key[rows, 2]

## Read step 2 CyclicQUV Optical Absorbance Data

filenames <-
  list.files(path = "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step2/",
```

```
           pattern = "\\.SPC$")

# Read Files

cq.abs.step2  <- lapply(filenames, function(i) {
  read.spc(paste(
    "./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step2/",
    i,
    sep = ""
  ))
})
```

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3209 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3151 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3094 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3094 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3379 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3209 > 1' in
coercion to 'logical(1)'

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coercion to 'logical(1)'

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coercion to 'logical(1)'

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coercion to 'logical(1)'

Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3209 > 1' in

17
```

```
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3209 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3209 > 1' in
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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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```

```
## coercion to 'logical(1)'

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## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

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## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'

## Warning in length(pos) == 1 && pos[[1]] == -1: 'length(x) = 3208 > 1' in
## coercion to 'logical(1)'
```

```r
# Combine resulting list into one hyperSpec object

cq.abs.step2 <-
  hyperSpec::collapse(cq.abs.step2[1:length(cq.abs.step2)])

# Add step data

cq.abs.step2@data$step <- 2
```

```
## Extract sample number from file name using sub (grep)
## to pull the sample number from the file name match to row in the keyfile

cq.abs.step2@data$sample <- filenames %>%
  sub(pattern = "-es02-ms02-mn01_uvvs01.SPC", replacement = "") %>%
  sub(pattern = "_", replacement = ".")

# Match material info from key file and add to hyperSpec object

rows <- cq.abs.step2@data$sample %>% pmatch(pet.key[, 1])
cq.abs.step2@data$material <- pet.key[rows, 2]
```

Lets check out the contents of each hyperSpec Object

`cq.abs.step0`

```
## hyperSpec object
##     6 spectra
##     7 data columns
##     3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (6 rows x 7 columns)
##     1. z: x/"a. u." [numeric] 0 0 ... 0
##     2. z.end: x/"a. u." [numeric] 0 0 ... 0
##     3. spc: A [AsIs matrix x 3201] 0.7163286 0.7948961 ... 0.1233116
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/sa25000_01-es(
##     5. step:  [numeric] 0 0 ... 0
##     6. sample:  [character] sa25000.01 sa25002.01 ... sa25010.01
##     7. material:  [character] B-Melinex243 B-Melinex238 ... B-TeteronU2L92W
```

`cq.abs.step1`

```
## hyperSpec object
##     54 spectra
##     7 data columns
##     3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (54 rows x 7 columns)
##     1. z: x/"a. u." [numeric] 0 0 ... 0
##     2. z.end: x/"a. u." [numeric] 0 0 ... 0
##     3. spc: A [AsIs matrix x 3201] 0.09173049 0.06935987 ... 0.1073754
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step1/sa25000_26-es(
##     5. step:  [numeric] 1 1 ... 1
##     6. sample:  [character] sa25000.26 sa25000.27 ... sa25010.34
##     7. material:  [character] B-Melinex243 B-Melinex243 ... B-TeteronU2L92W
```

`cq.abs.step2`

```
## hyperSpec object
##     48 spectra
##     7 data columns
##     3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (48 rows x 7 columns)
##     1. z: x/"a. u." [numeric] 0 0 ... 0
##     2. z.end: x/"a. u." [numeric] 0 0 ... 0
```

```
##     3. spc: A [AsIs matrix x 3201] -0.01496004 -0.02895853 ... 0.1794687
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step2/sa25000_27-es0
##     5. step:  [numeric] 2 2 ... 2
##     6. sample:  [character] sa25000.27 sa25000.28 ... sa25010.34
##     7. material:  [character] B-Melinex243 B-Melinex243 ... B-TeteronU2L92W
```

We'll put these all together

```r
# Combine cq.abs.step0s with step 1

cq.abs <- hyperSpec::collapse(cq.abs.step0, cq.abs.step1, cq.abs.step2)

cq.abs
```

```
## hyperSpec object
##     108 spectra
##     7 data columns
##     3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (108 rows x 7 columns)
##     1. z: x/"a. u." [numeric] 0 0 ... 0
##     2. z.end: x/"a. u." [numeric] 0 0 ... 0
##     3. spc: A [AsIs matrix x 3201] 0.7163286 0.7948961 ... 0.1794687
##     4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/sa25000_01-es0
##     5. step: step [numeric] 0 0 ... 2
##     6. sample: sample [character] sa25000.01 sa25002.01 ... sa25010.34
##     7. material: material [character] B-Melinex243 B-Melinex238 ... B-TeteronU2L92W
```

```r
# Divide by sample thickness for Abs/cm

t.melinex243 <- 0.005
t.melinex238 <- 0.0127
t.melinex626 <- 0.0127
t.melinex618 <- 0.0127
t.teteronu2 <- 0.005
t.teteronu2l92w <- 0.0125

for (i in 1:length(cq.abs@data$material)) {
  if (cq.abs@data$material[i] == "B-Melinex243") {
    cq.abs[i] <- cq.abs[i] / t.melinex243
  }
  if (cq.abs@data$material[i] == "B-Melinex238") {
    cq.abs[i] <- cq.abs[i] / t.melinex238
  }
  if (cq.abs@data$material[i] == "A-Melinex626") {
    cq.abs[i] <- cq.abs[i] / t.melinex626
  }
  if (cq.abs@data$material[i] == "A-Melinex618") {
    cq.abs[i] <- cq.abs[i] / t.melinex618
  }
  if (cq.abs@data$material[i] == "B-TeteronU2") {
    cq.abs[i] <- cq.abs[i] / t.teteronu2
  }
  if (cq.abs@data$material[i] == "B-TeteronU2L92W") {
```

```
    cq.abs[i] <- cq.abs[i] / t.teteronu2l92w
  }
}

cq.abs
```

5.1.2.6 Utilizing spectral arithmetric to change ordinate axis

```
## hyperSpec object
##    108 spectra
##    7 data columns
##    3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (108 rows x 7 columns)
##    1. z: x/"a. u." [numeric] 0 0 ... 0
##    2. z.end: x/"a. u." [numeric] 0 0 ... 0
##    3. spc: A [AsIs matrix x 3201] 143.26572 62.59025 ... 14.3575
##    4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/sa25000_01-es(
##    5. step: step [numeric] 0 0 ... 2
##    6. sample: sample [character] sa25000.01 sa25002.01 ... sa25010.34
##    7. material: material [character] B-Melinex243 B-Melinex238 ... B-TeteronU2L92W
```

```
# Remove erroneous points (negative)

`cq.abs`[[`cq.abs` < 0]] <- NA

cq.abs
```

```
## hyperSpec object
##    108 spectra
##    7 data columns
##    3201 data points / spectrum
## wavelength: lambda/nm [numeric] 200.0 200.5 ... 1800
## data:  (108 rows x 7 columns)
##    1. z: x/"a. u." [numeric] 0 0 ... 0
##    2. z.end: x/"a. u." [numeric] 0 0 ... 0
##    3. spc: A [AsIs matrix x 3201] 143.26572 62.59025 ... 14.3575 + NA
##    4. filename: filename [character] ./data/pet_unstab_cyclic_quv/Cary/CyclicQUV/step0/sa25000_01-es(
##    5. step: step [numeric] 0 0 ... 2
##    6. sample: sample [character] sa25000.01 sa25002.01 ... sa25010.34
##    7. material: material [character] B-Melinex243 B-Melinex238 ... B-TeteronU2L92W
```

5.1.2.6.1 Better plotting using ggplot2 graphics

Optical Absorbance Spectra - CyclicQUV
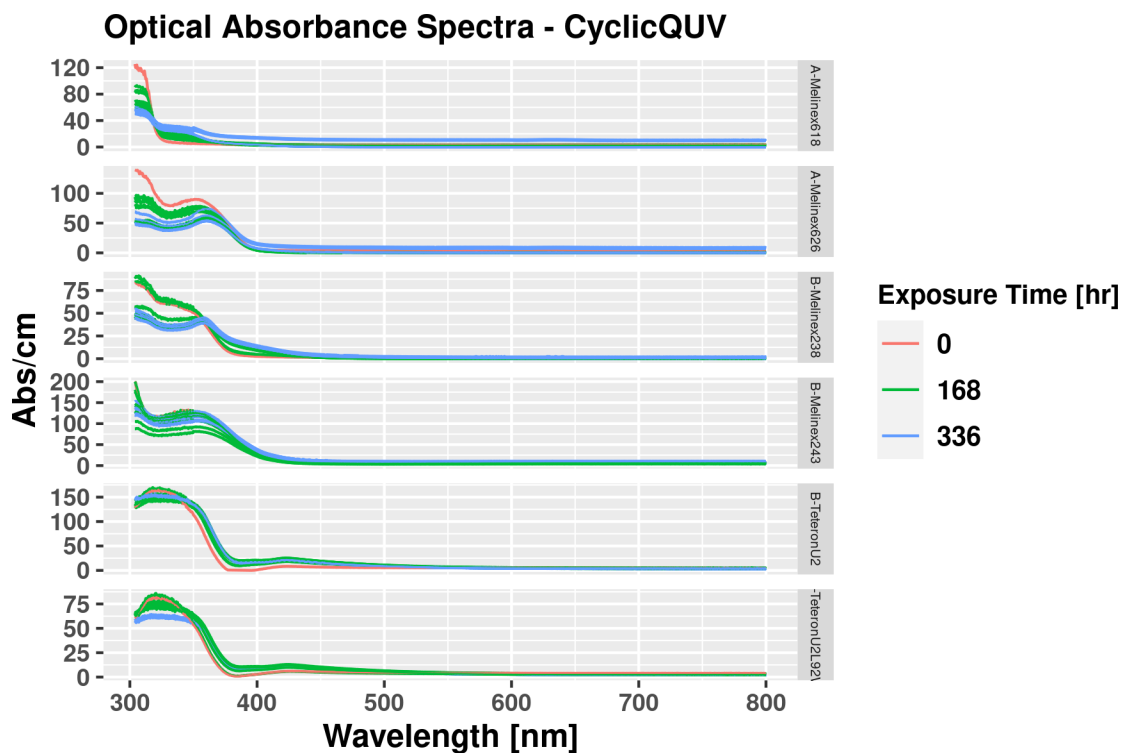
5.1.2.7 Peak Information extraction We can directly address the intensity value at a specific wavelength

```
spec[2,,460]@data$spc
```

```
##            460
## [1,] 266.9985
```

Using this concept,

- we can also find full width at half max
  - by approximating the wavelengths
  - at half the intensity of the peak

```
lower <-
  approx(spec[2, , 330 ~ 460]$spc, spec[2, , 330 ~ 460]@wavelength,
         xout = c(spec[2, , 460]$spc / 2))
lower
```

```
## $x
## [1] 133.4993
##
## $y
## [1] 383.7909
```

```
upper <-
  approx(spec[2, , 460 ~ 600]$spc, spec[2, , 460 ~ 600]@wavelength,
         xout = c(spec[2, , 460]$spc / 2))
upper
```

```
## $x
## [1] 133.4993
##
```

```
## $y
## [1] 506.0615
```

```
fwhm <- upper$y - lower$y
fwhm
```

```
## [1] 122.2706
```

Imagine this as a function that could operate on multiple spectra

```r
fwhm.spc <- function(spec, peak.wl, lower.bound, upper.bound) {
  peak.wl <- as.numeric(peak.wl)

  lower <- approx(spec[, , lower.bound ~ peak.wl]$spc,
                  spec[, , lower.bound ~ peak.wl]@wavelength,
                  xout = c(spec[, , peak.wl]$spc / 2))

  upper <- approx(spec[, , peak.wl ~ upper.bound]$spc,
                  spec[, , peak.wl ~ upper.bound]@wavelength,
                  xout = c(spec[, , peak.wl]$spc / 2))

  fwhm <- upper$y - lower$y
  center <- mean(c(upper$y, lower$y))
  skew <- 1 - (upper$y - peak.wl) / (fwhm / 2)

  return(c(fwhm, center, skew))
}
```

Let's try it

```r
#Start a data frame to hold the data

ex320data <- read.csv("./data/petpilot-key.csv")

ex320data$Em.Peak <- NA
ex320data$Em.Peak.int <- NA
ex320data$Em.Peak.fwhm <- NA
ex320data$Em.Peak.center <- NA
ex320data$Em.Peak.skew <- NA
ex320data$Em.Peak.skew.mag <- NA


# We'll use a for loop to run each spectrum in the hyperSpec Object
row <- 1

for (i in 1:length(spec)) {
  # Define temporary holder for spectrum of interest

  temp <- spec[i]

  #Define the upper and lower bounds for the approx function

  lower.bound <- min(temp@wavelength)
  upper.bound <- max(temp@wavelength)

  # Find the maximum value in the region of interest
  peak <- max(temp[, , 450 ~ 470])
```

```
    ex320data$Em.Peak.int[row] <- peak

    # Find the peak wavelength

    peak.out <-
      approx(temp[, , 450 ~ 470]$spc, temp[, , 450 ~ 470]@wavelength,
             xout = max(temp[, , 450 ~ 470]))
    peak.wl <- ifelse(is.na(peak.out$y) == TRUE, 450, peak.out$y)
    ex320data$Em.Peak[row] <- peak.wl

    # Run our function

    spec.data <-
      fwhm.spc(temp, as.numeric(peak.wl), lower.bound, upper.bound)

    # Store values in data frame

    ex320data$Em.Peak.fwhm[row] <- spec.data[1]
    ex320data$Em.Peak.center[row] <- spec.data[2]
    ex320data$Em.Peak.skew[row] <- spec.data[3]
  row <- row + 1
}
```

Check the result

```
head(ex320data)
```

```
##        Sample             Material.Type Exposure.Type Exposure.Step
## 1 sa19601.00 hydrolytically.stabilized       baseline             0
## 2 sa19601.01 hydrolytically.stabilized       dampheat             1
## 3 sa19601.02 hydrolytically.stabilized       dampheat             2
## 4 sa19601.03 hydrolytically.stabilized       dampheat             3
## 5 sa19601.04 hydrolytically.stabilized       dampheat             4
## 6 sa19601.05 hydrolytically.stabilized       dampheat             5
##   Exposure.Time Total.UV.Dose Em.Peak Em.Peak.int Em.Peak.fwhm Em.Peak.center
## 1             0             0  450.00    22.99323           NA             NA
## 2           168             0  460.00   266.99850    122.27058       444.9262
## 3           336             0  458.93   339.14621     92.05087       458.9813
## 4           504             0  460.00   386.45648     93.64712       460.1745
## 5           672             0  461.06   408.56882     90.03078       461.9307
## 6           840             0  461.96   509.58521     87.02260       463.3233
##   Em.Peak.skew Em.Peak.skew.mag
## 1           NA               NA
## 2  0.246564551               NA
## 3 -0.001115496               NA
## 4 -0.003725775               NA
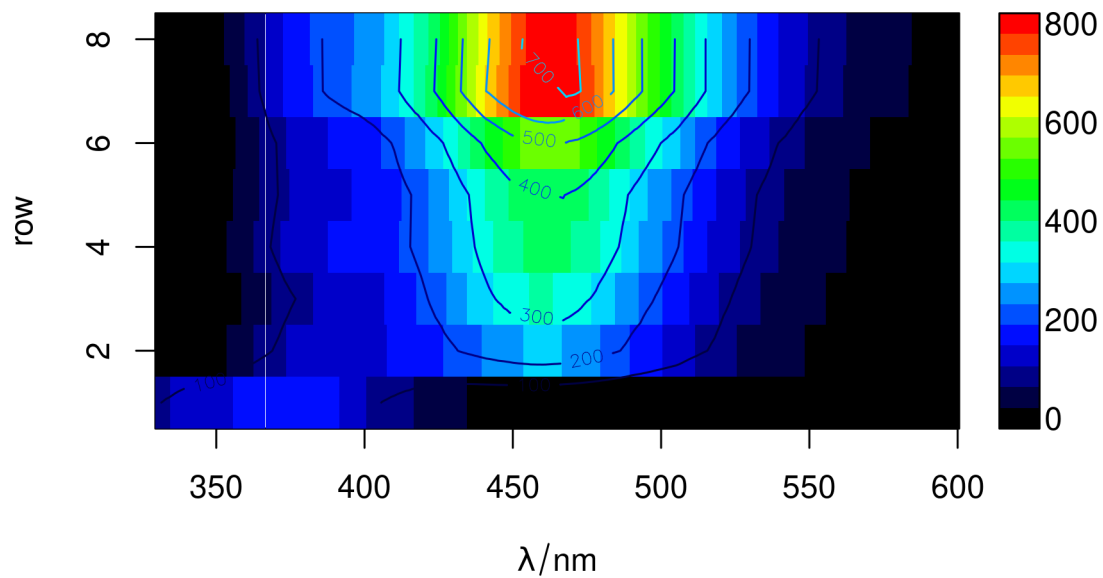## 5 -0.019342267               NA
## 6 -0.031332943               NA
```

5.1.2.8 Other plots

```
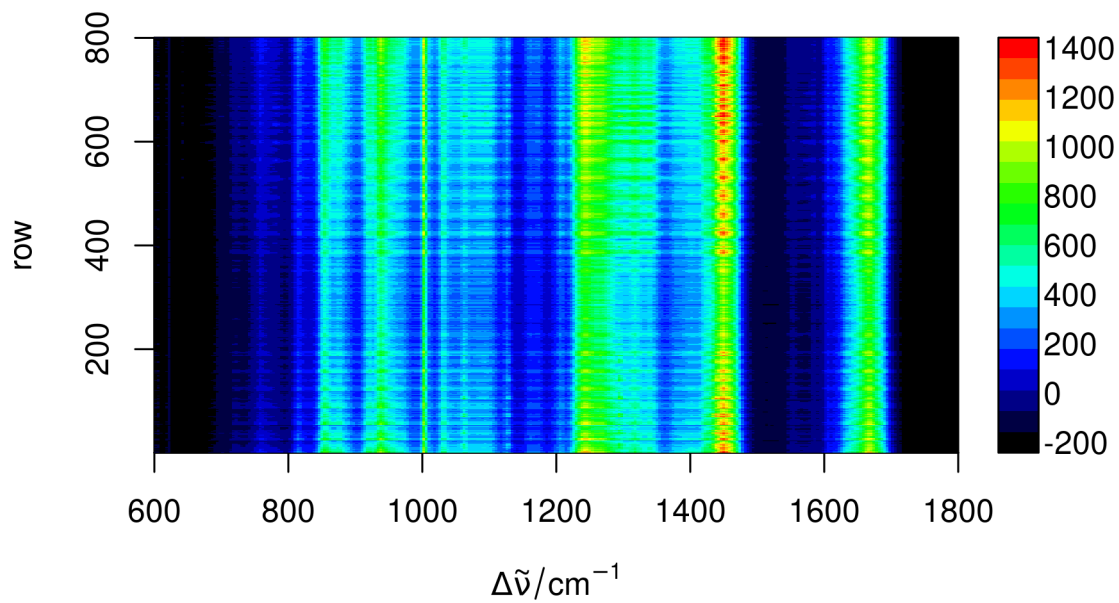plotmat(spec)
plotmat(spec, contour = TRUE, add = TRUE)
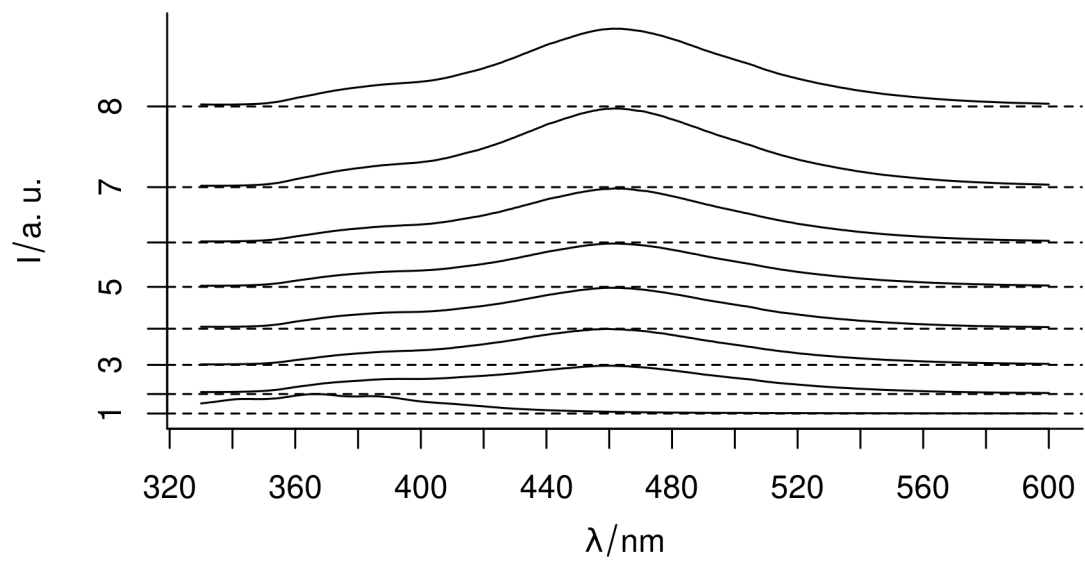```

**5.1.2.8.1    Matrix Plot - Fluorescence Data**



```
plotmat(ir.spc)
```

5.1.2.8.2   Matrix Plot - IR Data


```
plotspc(spec, stacked = TRUE)
```

5.1.2.8.3   Stacked Spectra

5.1.2.9 Summary

5.1.2.9.1 hyperSpec

- hyperSpec is a powerful R package for handling and manipulating spectral data in R