Practical guide on dissolved organic matter (DOM) optic

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2016-08-31

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Chapter 1

Introduction and motivations

Dissolved organic matter (DOM) plays fundamental roles in the ecology of aquatic ecosystems. Physical and chemical characteristics of the DOM transiting in aquatic ecosystems are important parameters that drive their functioning at different levels. For example, dissolved organic carbon (DOC) is the major fraction of the DOM pool and represents the main source of metabolic substrates for heterotrophic bacteria and influences the composition of aquatic microbial communities (Findlay2003). Additionally, the chromophoric fraction of the DOM pool (CDOM) is a major driver of underwater light characteristics (Kirk1994) which modulate many bio-optical processes such as primary production (Thrane2014, Seekell2015) and also constitute a natural screen protecting aquatic organisms against harmful ultraviolet (UV) radiations (Boily2012).

- DOM is a complex mixture containing thousands of different chemical compounds (ref).
- Traditional chemical analysis used to characterize DOM are expensive.
- Optical methods have been developed.
- Why this project? Already few good books (Lakowicz, 2006)
- Need for unified way to present stuff with correct citation.

1.1 References

Chapter 2

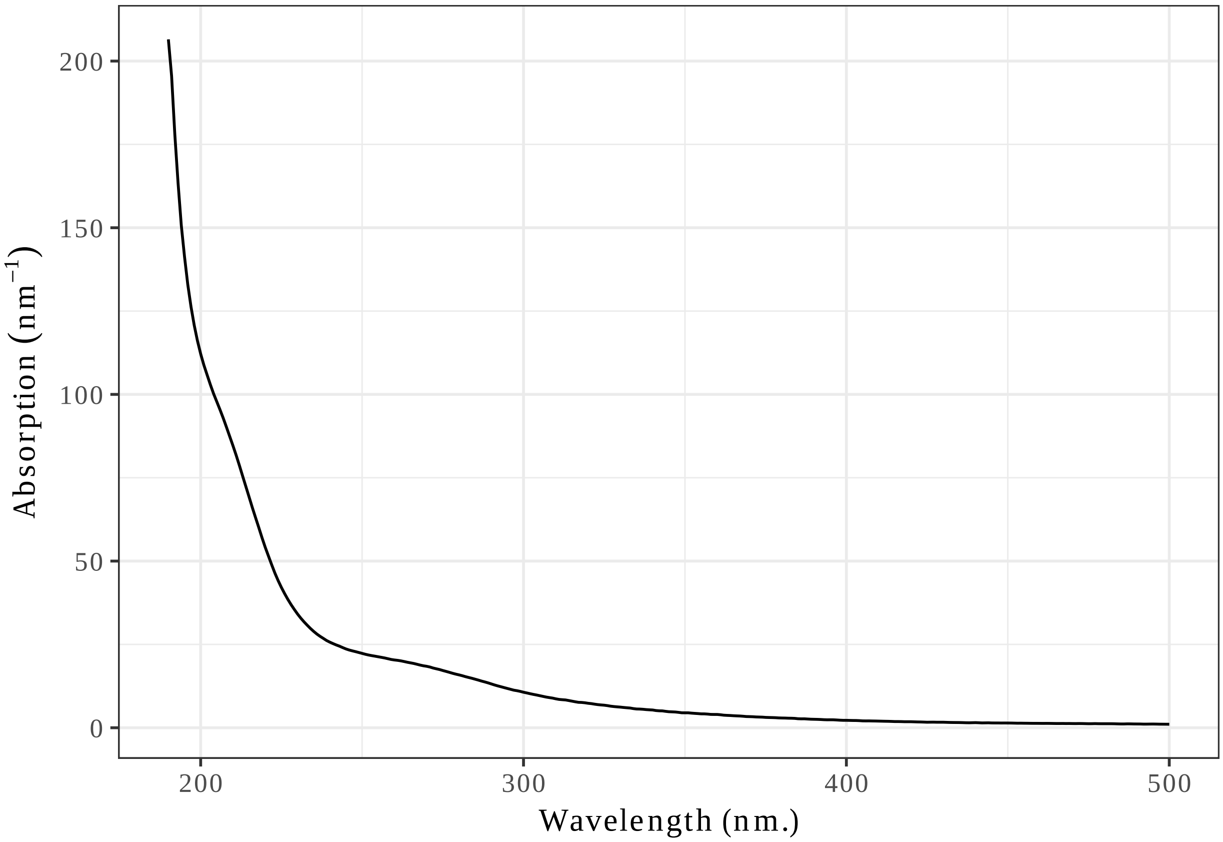
Absorbance

```
library(cdom)
data(spectra)

spectra <- spectra %>% filter(wavelength <= 500)

p <- ggplot(spectra, aes(x = wavelength, y = spc1)) +
  geom_line() +
  xlab("Wavelength (nm.)") +
  ylab(bquote(Absorption~(nm^{-1})))

p
```



2.1 Absorbance vs absorption

$$a_{\mathrm{CDOM}}(\lambda) = \frac{A(\lambda) \times 2.303}{L}$$

2.2 Spectral slopes

- Exponential shape.
- Cite the 3 references and why (Stedmon and Markager, 2001; Jerlov, 1968; Bricaud et al., 1981).

$$a_{\mathrm{CDOM}}(\lambda) = a_{\mathrm{CDOM}}(\lambda 0)e^{-S(\lambda - \lambda 0)} + K$$

Where $a_{\mathrm{CDOM}}(\lambda)$ is the absorption coefficient (m^{-1}), λ is the wavelength (nm), $\lambda 0$ is a reference wavelength (nm), K is a background constant (m^{-1}) accounting for scatter in the cuvette and drift of the instrument and S is the spectral slope (nm^{-1}) that describes the approximate exponential rate of decrease of absorption with increasing wavelength. Higher slopes indicate a more rapid decrease in absorption with increasing wavelength. The S parameter is frequently used as a proxy for tracing photochemical and microbial-induced changes of CDOM [Moran2000,Twardowski2004,Helms2013] or to determine its origin [Stedmon2001].

- Nonlinear fit

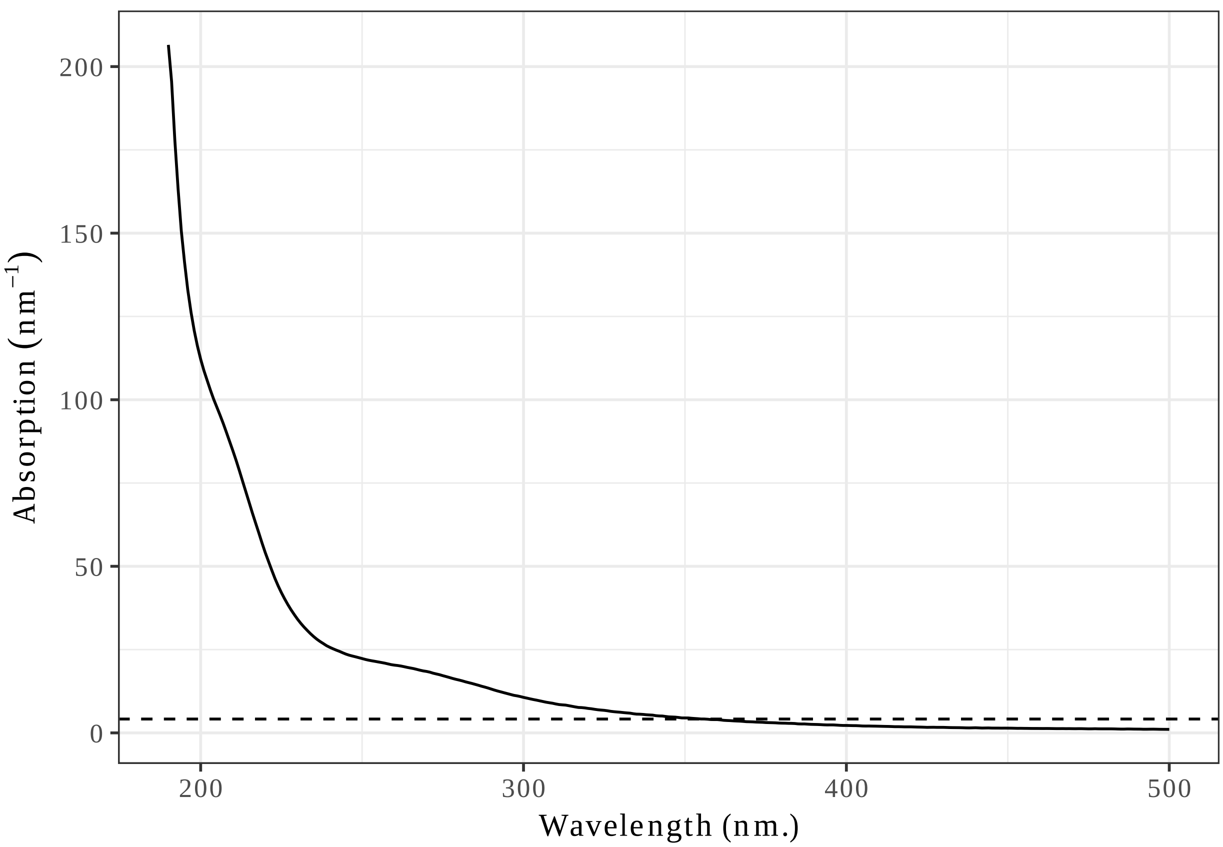
```
mod <- nls(spc1 ~ a0 * exp(-s * (wavelength - 350)) + k,
           data = spectra,
           start = list(a0 = 5, s = 0.02, k = 0))
```

```r
summary(mod)
```

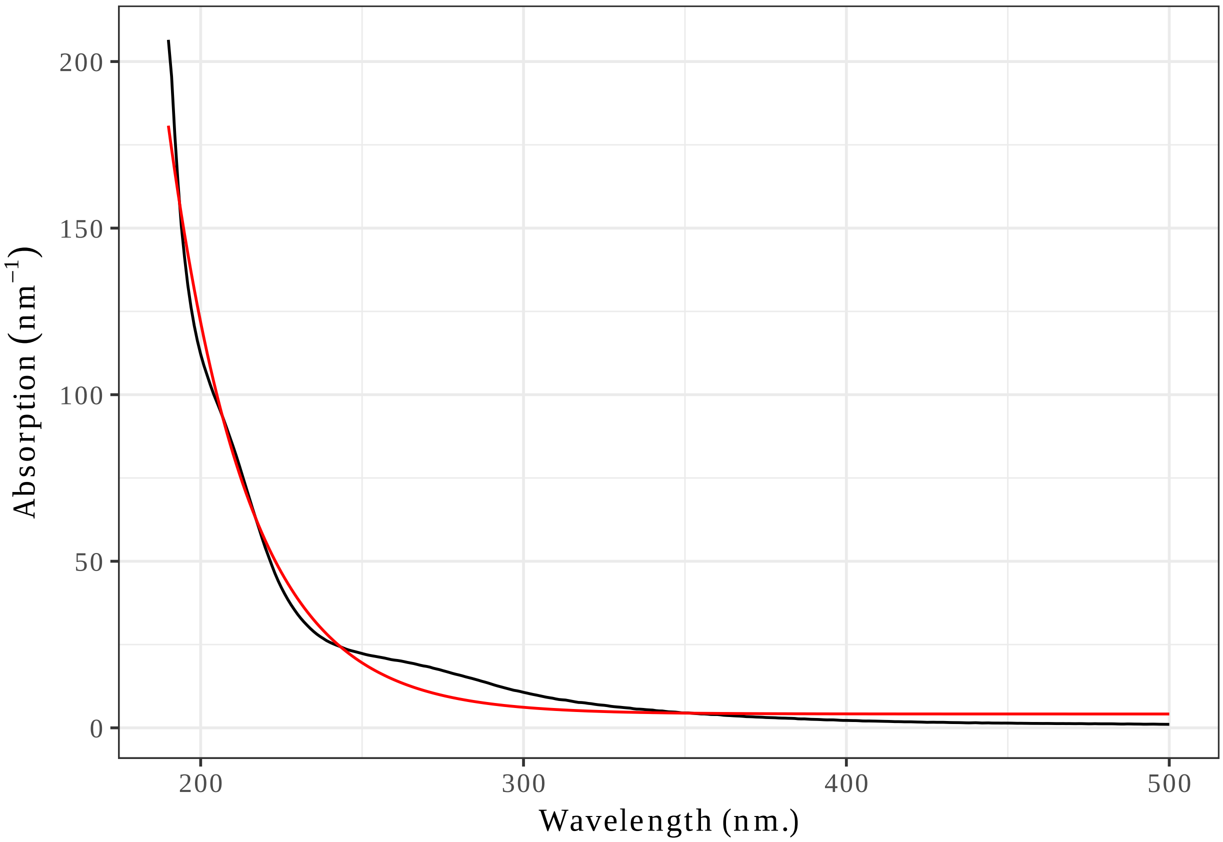
```
##
## Formula: spc1 ~ a0 * exp(-s * (wavelength - 350)) + k
##
## Parameters:
##     Estimate Std. Error t value Pr(>|t|)
## a0 0.2624416  0.0237320   11.06   <2e-16 ***
## s  0.0406974  0.0005989   67.96   <2e-16 ***
## k  4.1539547  0.2871120   14.47   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.187 on 308 degrees of freedom
##
## Number of iterations to convergence: 16
## Achieved convergence tolerance: 7.177e-06
```

The value of S is 0.0406974 meaning that absorption is decreasing at a rate of 0.0406974 m^{-1} for each increase of 1 nm.

- k parameter (scattering, introduced by Stedmon and Markager (2001))



```
p + geom_line(aes(y = predict(mod)), col = "red")
```



2.3 Metrics

- $S_{300-600}$ linked to DOM molecular weight (Stedmon and Nelson, 2015).

2.3.1 Slope ratio

The slope ratio (S_R) is defined as the ratio between $S_{275-295}$ and $S_{350-400}$ (Helms et al., 2008).

According to Helms et al. (2008):

> By calculating the ratio of the slope of the shorter wavelength region (275–295 nm) to that of the longer wavelength region (350–400 nm), a dimensionless parameter called "slope ratio" or S_R is defined. This approach avoids the use of spectral data near the detection limit of the instruments used, and focuses on absorbance values that shift dramatically during estuarine transit and photochemical alteration of CDOM.

2.4 References

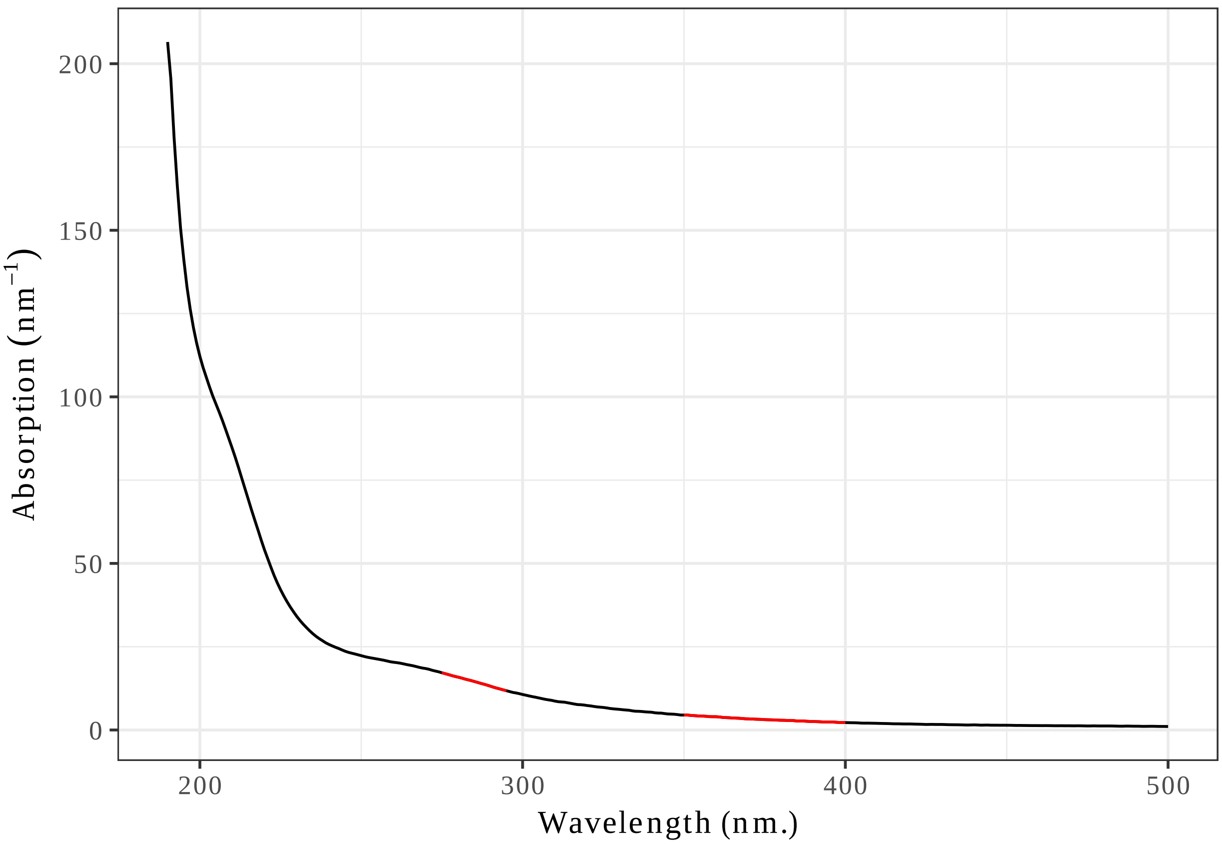


Figure 2.1: Graph showing the spectral range used to calculate the slope ratio.

Chapter 3

Fluorescence

3.1 Introduction

- What is a EEM
- Principal metrics (BIX, HIX, FI, etc.)
- PARAFAC

Bibliography

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Helms, J. R., Stubbins, A., Ritchie, J. D., Minor, E. C., Kieber, D. J., and Mopper, K. (2008). Absorption spectral slopes and slope ratios as indicators of molecular weight, source, and photobleaching of chromophoric dissolved organic matter. *Limnology and Oceanography*, 53(3):955–969.

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