Introduction to USGSHydroOpt

Samuel Christel[1] and Steve Corsi[1]

[1] *United States Geological Survey*

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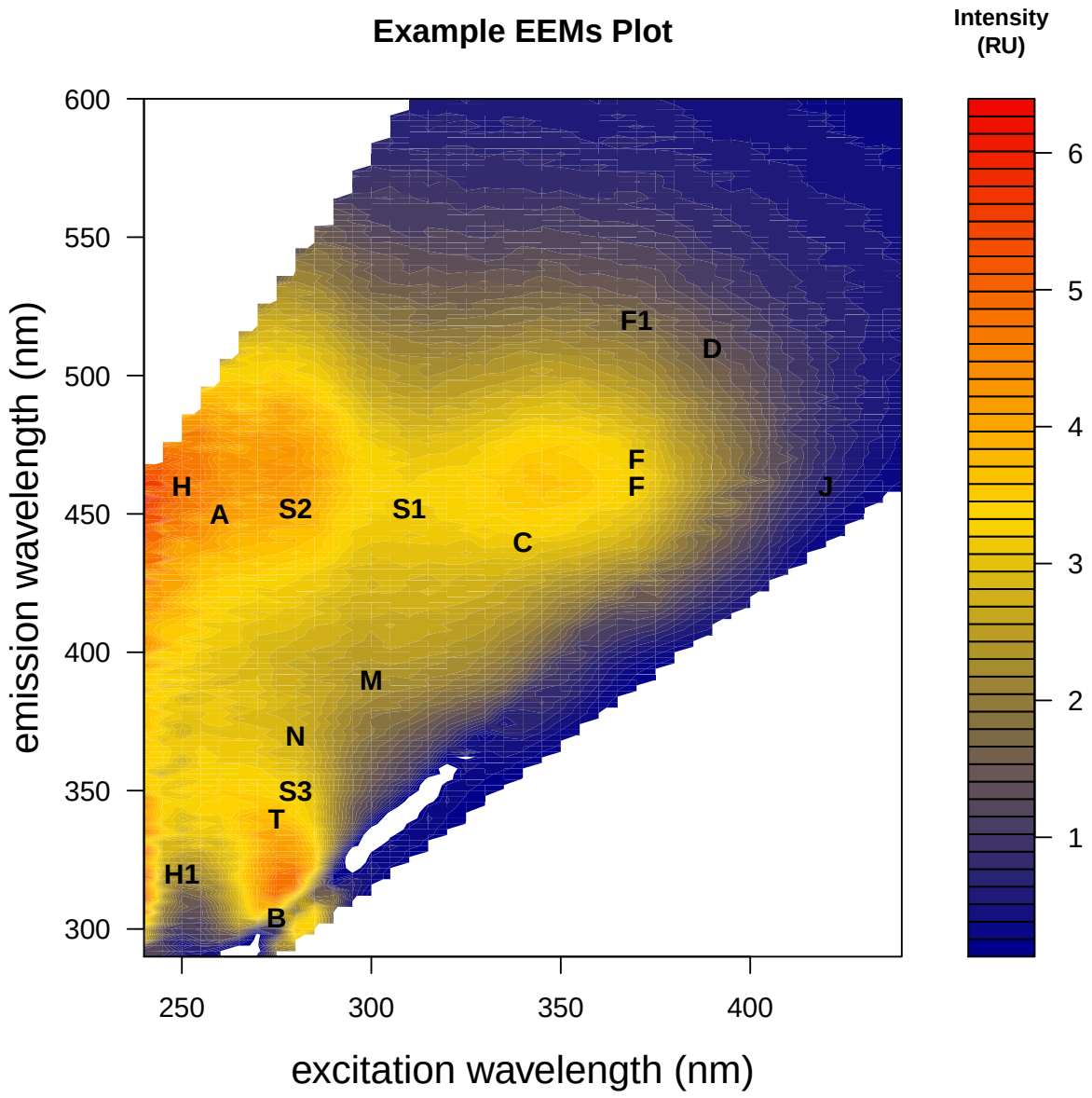
1 Introduction to USGSHydroOpt

The USGSHydroOpt package was created to streamline the process of creating optical summary variables and excitation-emission (EEMs) plots for absorbance and fluoresence data collected from various freshwater sources. Examples of optical summary variables that can be produced with this package include various absorbance peaks, The functions in this package were designed to operate on dataframes with a standard data structures. This package is not amenable to dataframes or arrays that do not fit the prescribed formats. The example dataframes and array in this package illustrate exactly how data structures should be formatted, and the examples illustrate how the functions operate on the data structures. Depicted below is an example of an EEMs plot produced with this package.




```
NULL
```

2 Data Formats Required for USGS HydroOpt

The functions contained in USGSHydroOpt operate on dataframes with defined structures. Users interested in using USGSHydroOpt should format dataframes according to the structures defined in this section.

2.1 Absorbance Data

Absorbance data used by functions in USGSHydroOpt should be formatted such that each sample occupies a column, and one column contains the wavelength (nm) for which the absorbance measurement was mea-

sured (*See example Table 2.1 below*). The column with the wavelengths in Table 2.1 does not need to be called "wavelengths," as it is named in the example dataframe below. Since this package was developed primarily for USGS activities, the default for naming samples is "gr" then the sample number. This convention was started by the USGS California Water Sciences Center (CA WSC) and the USGS Wisconsin Water Science Center (WI WSC) follows the same naming convention to ensure standardization.

```
     gr13307    gr13351    gr13353    gr13357 wavelengths
1  0.0001296 -0.0003505 -0.0003480 -0.0002695         750
2 -0.0002367  0.0000305 -0.0000915 -0.0001407         749
3 -0.0001582 -0.0004900 -0.0006325 -0.0001534         748
4 -0.0004642 -0.0000105 -0.0000932 -0.0000245         747
5 -0.0002551 -0.0000653  0.0000841 -0.0001615         746
6 -0.0001842 -0.0002135  0.0002082  0.0001429         745
```

2.2 Fluoresence Data

Fluoresence data used by functions in USGSHydroOpt should also be formatted such that each sample occupies a column, and one column contains the excitation emission wavelength pairs (nm) for which the fluoresence measurment was measured (*See example Table 2.2 below*). The column with the excitation emission pairs in Table 2.2 does not need to be called "Wavelength.Pairs," as it is in the example dataframe below. Again since this package was developed for USGS activities, the default sample naming convention is "gr" followed by the sample number.

```
  Wavelength.Pairs gr13307 gr13308  gr13351  gr13352
1          240/290 0.09457 0.05358 -0.07268 -0.19368
2          240/292 0.07386 0.09194  0.45433  0.39722
3          240/294 0.08116 0.09930  0.49135  0.37943
4          240/296 0.12013 0.09138 -0.12248  0.09239
5          240/298 0.15264 0.15428  0.54694  0.14980
6          240/300 0.16467 0.13010  0.43319  0.33064
```

2.3 Spectral Slopes Data

Information on the upper and lower wavelength (nm) for which a spectral slope should be calculated needs to be stored in a dataframe if USGSHydroOpt is used. The dataframe should contain exactly three columns. The first column should contain the upper wavelength, the second column should contain the lower wavelength, and the third column should contain the name of the spectral slope being calculated (*See example Table 2.3 below*). The columns in Table 2.3 need to be in this exact order, although the names of the columns may be different. The data types for each column are integer, integer, and character, respectively. More spectral slopes can be added to the table than specified in the example dataframe below.

```
  wvlngth1 wvlngth2       Name
1      275      290 Sag275_295
2      290      350 Sag290_350
3      350      400 Sag350_400
4      412      676 Sag412_676
```

2.4 Optical Summary Data

This is the dataframe that contains many of the summary optical variables that can be produced using functions in USGSHydroOpt (*See example Table 2.4a below*). The functions in USGSHydroOpt calculate summary optical variables and add to a dataframe formatted according to Table 2.4a below. The example dataframe below is how the WI WSC stores optical summary variables. Note that this dataframe can contain other columns with metadata, for example, the sample data and time, the sample ID, or whether or not the sample went through QA/QC.

```
  GRnumber          B      T      A       J FI_2005    A254
1  gr13307  0.050997 0.1826 0.4553 0.03705   1.639 0.05228
2  gr13351 -0.245602 0.4085 3.0783 0.19110   1.456 0.43531
3  gr13353 -0.175220 0.7794 6.8624 0.56309   1.523 0.68274
4  gr13357  0.111561 0.2691 0.9451 0.06969   1.572 0.08698
5  gr13360 -0.001569 0.4593 2.8254 0.37231   1.563 0.28605
6  gr13363  0.052137 0.4892 1.9518 0.19098   1.583 0.19283
```

However, also note that summary optical variable names in the dataframe must be identical to those specified in Table 2.4b below.

```
 [1] "OB1"         "OB2"         "OB3"         "S1.50"
 [5] "S2.50"       "S3.50"       "S1.25"       "S2.25"
 [9] "S3.25"       "Mrange.25"   "Mrange.50"   "B"
[13] "T"           "M"           "A"           "C"
[17] "N"           "D"           "F"           "J"
[21] "S1"          "S2"          "S3"          "H1"
[25] "H2"          "F1"          "F2"          "W"
[29] "LT1"         "LT2"         "LT3"         "LA"
[33] "HIX_2002"    "FI_2005"     "FI_2001"     "FreshI"
[37] "A254"        "A275"        "A280"        "A290"
[41] "A295"        "A350"        "A370"        "A400"
[45] "A412"        "A440"        "A488"        "A510"
[49] "A532"        "A555"        "A650"        "A676"
[53] "A715"        "Sag275_290"  "Sag290_350"  "Sag350_400"
[57] "Sag412_676"  "Aresids"
```

2.5 Excitation-Emission (EEMs) Peak Data

The EEMs peak data contains three columns listing the name of a characterized EEM peak along with the corresponding wavelengths (nm) (*See example Table 2.5 below*). The first column, in Table 2.5, "Peak," contains the name of the characterized EEM peak. The next two columns in Table 2.5 contain the excitation and emission wavelengths (nm) at which a given peak occurs. The column names must be identical to those displayed in the example below, although the order of the columns can be different.

```
  Peak ExCA EmCA
1    B  275  304
2    T  275  340
3    M  300  390
4    A  260  450
```

```
5     C  340  440
6     N  280  370
7     D  390  510
8     F  370  460
9     J  420  460
10   S1  310  452
11   S2  280  452
12   S3  280  350
13    H  250  460
14   H1  250  320
15    F  370  470
16   F1  370  520
```

2.6 Optical Ratio and Signals Data

This dataframe contains one column called "ratioSignals" that contains all of the summary optical variables currently identified by the WI WSC (*See example Table 2.6 below*). Note that these are the same variables as those listed in Table 2.4b. The first column must contain the various "ratioSignals" that the user desires, although the column name need not be "ratioSignals"

```
   ratioSignals keep
1           OB1   NA
2           OB2   NA
3           OB3   NA
4         S1.50   NA
5         S2.50   NA
6         S3.50   NA
7         S1.25   NA
8         S2.25   NA
9         S3.25   NA
10    Mrange.25   NA
11    Mrange.50   NA
12            B   NA
13            T   NA
14            M   NA
15            A   NA
16            C   NA
17            N   NA
18            D   NA
19            F   NA
20            J   NA
21           S1   NA
22           S2   NA
23           S3   NA
24           H1   NA
25           H2   NA
26           F1   NA
27           F2   NA
```

```
28            W   NA
29          LT1   NA
30          LT2   NA
31          LT3   NA
32           LA   NA
33     HIX_2002   NA
34      FI_2005   NA
35      FI_2001   NA
36       FreshI   NA
37         A254    1
38         A275    1
39         A280    1
40         A290    1
41         A295    1
42         A350    1
43         A370    1
44         A400    1
45         A412   NA
46         A440   NA
47         A488   NA
48         A510   NA
49         A532   NA
50         A555   NA
51         A650   NA
52         A676   NA
53         A715   NA
54   Sag275_290    1
55   Sag290_350    1
56   Sag350_400    1
57   Sag412_676    1
58      Aresids   NA
```

2.7 Optical Signals Data

This dataframe is similar to "ratioSignals" except it provides more metadata about peaks characterized for EEMs plots. The dataframe should contain six columns (*See example Table 2.7 below*). The first column in Table 2.7, "Peak," contains the name of the characterized EEM peak. The next two columns, "Ex1" and "Ex2," contain the excitation wavelength range (nm) for a given peak. "Ex1" is the lower wavelength and "Ex2" is the upper wavelength for the excitation wavelength range (nm) for a given peak. Similarily, "Em1" and "Em2" contain the emission wavelength range (nm) for a given peak. The final column, "Source," lists the source that characterized the peak. The last column, "Source," is not required. The user must exactly replicate the column names in Table 2.7 in order for the code in USGSHydroOpt to run.

```
        Peak Ex1 Ex2 Em1 Em2                  Source
1        OB1 360  NA 410 598           Hartel Turner
2        OB2 360  NA 436 436           Hartel Turner
3        OB3 365  NA 400 550         Hagedorn Turner
4      S1.50 310  NA 402 502                Sniffer
```

```
5       S2.50 280  NA 402 502                    Sniffer
6       S3.50 280  NA 310 390                    Sniffer
7       S1.25 310  NA 427 477                    Sniffer
8       S2.25 280  NA 427 477                    Sniffer
9       S3.25 280  NA 330 370                    Sniffer
10 Mrange.25 300  NA 365 415                       test
11 Mrange.50 300  NA 340 440                       test
12          B 275  NA 304  NA                         CA
13          T 275  NA 340  NA                         CA
14          M 300  NA 390  NA                         CA
15          A 260  NA 450  NA                         CA
16          C 340  NA 440  NA                         CA
17          N 280  NA 370  NA                         CA
18          D 390  NA 510  NA                         CA
19          F 370  NA 460  NA                         CA
20          J 420  NA 460  NA                         CA
21         S1 310  NA 452  NA                         CA
22         S2 280  NA 452  NA                         CA
23         S3 280  NA 350  NA                         CA
24         H1 250  NA 460  NA                   Ohno2002
25         H2 250  NA 320  NA                   Ohno2002
26         F1 370  NA 470  NA Cory and McKnight, 2005
27         F2 370  NA 520  NA Cory and McKnight, 2005
28          W 255 290 302 350
29        LT1 250  NA 340  NA
30        LT2 260  NA 340  NA
31        LT3 240  NA 340  NA
32         LA 240  NA 440  NA
```

2.8 3-Dimensional Excitation-Emission Array

A 3-D array with fluoresence data is used by many of the functions in USGSHydroOpt. The first dimension contains the excitation wavelengths (nm) as data type character at which a given fluoresence measurement was made. The second dimension contains the emission wavelengths (nm) as data type character at which a given fluoresence measurement was made. The third dimension contains the sample numbers as data type character for a given observation. The user must ensure that the third dimension of the array are sample numbers. Again, in this example the default ”gr” followed by the sample number is used as a naming convention for samples.

To view the headers for each dimension using the following commands in R consider the example 3-D EEM array included with the USGSHydroOpt Package:

```
#this command shows the excitation wavelengths (nm)
colnames(a)
```

```
  [1] "290" "292" "294" "296" "298" "300" "302" "304" "306"
 [10] "308" "310" "312" "314" "316" "318" "320" "322" "324"
 [19] "326" "328" "330" "332" "334" "336" "338" "340" "342"
```

```
 [28] "344" "346" "348" "350" "352" "354" "356" "358" "360"
 [37] "362" "364" "366" "368" "370" "372" "374" "376" "378"
 [46] "380" "382" "384" "386" "388" "390" "392" "394" "396"
 [55] "398" "400" "402" "404" "406" "408" "410" "412" "414"
 [64] "416" "418" "420" "422" "424" "426" "428" "430" "432"
 [73] "434" "436" "438" "440" "442" "444" "446" "448" "450"
 [82] "452" "454" "456" "458" "460" "462" "464" "466" "468"
 [91] "470" "472" "474" "476" "478" "480" "482" "484" "486"
[100] "488" "490" "492" "494" "496" "498" "500" "502" "504"
[109] "506" "508" "510" "512" "514" "516" "518" "520" "522"
[118] "524" "526" "528" "530" "532" "534" "536" "538" "540"
[127] "542" "544" "546" "548" "550" "552" "554" "556" "558"
[136] "560" "562" "564" "566" "568" "570" "572" "574" "576"
[145] "578" "580" "582" "584" "586" "588" "590" "592" "594"
[154] "596" "598" "600"

#this command shows the emission wavelengths (nm)
rownames(a)

 [1] "240" "245" "250" "255" "260" "265" "270" "275" "280"
[10] "285" "290" "295" "300" "305" "310" "315" "320" "325"
[19] "330" "335" "340" "345" "350" "355" "360" "365" "370"
[28] "375" "380" "385" "390" "395" "400" "405" "410" "415"
[37] "420" "425" "430" "435" "440"

#this command shows the emission wavelengths (nm), only the first 20 shown for
names(a[1,1,])[1:20]

 [1] "gr13307" "gr13308" "gr13351" "gr13352" "gr13353"
 [6] "gr13354" "gr13357" "gr13358" "gr13360" "gr13361"
[11] "gr13362" "gr13363" "gr13364" "gr13365" "gr13374"
[16] "gr13375" "gr13433" "gr13434" "gr13435" "gr13439"
```

The user should be aware of **two important caveats**: (1) There should rarely be emission wavelengths below the excitation wavelength for a given fluoresence reading. Where this occurs an NA will be found in the 3-D EEMs array. (2) Intensities at an emission wavelength that is two times the excitation wavelength will be influence by second order Rayleigh scatter.

2.9 Creating a 3-Dimensional Excitation-Emission Array

In Section 2.8 the format of 3-D arrays of fluoresence data that can be used with USGSHydroOpt was discussed. USGSHydroOpt can also be used to produce such arrays given the appropriate input fluoresence dataframe. Below is an example of how USGSHydroOpt is used to accomplish this task:

```
#set an arbitrary data frame (df) as dfFluor (the example fluoresence dataframe
df <- dfFluor

#define the column in dfFluor
ExEm <- "Wavelength.Pairs"
```

```
#run the VectorizedTo3DArray function from USGSHydroOpt that creates a 3-D EEMs
aTest <- VectorizedTo3DArray(df,ExEm)
```

In the example above, dfFluor is formatted according to the fluoresence dataframe discussed in Section 2.2.