Introduction to the EGRET package

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1 Introduction to Exploration and Graphics for RivEr Trends (EGRET)

For information on getting started in R, downloading and installing the package, see Appendix 1: (A).

Exploration and Graphics for RivEr Trends (EGRET): An R-package for the analysis of long-term changes in water quality and streamflow.

EGRET includes statistics and graphics for streamflow history, water quality trends, and the modeling algorithm Weighted Regressions on Time, Discharge, and Season (WRTDS). The best way to learn about the WRTDS approach and to see examples of its application to multiple large data sets is to read two journal articles. Both are available, for free, from the journals in which they were published.

The first relates to nitrate and total phosphorus data for 9 rivers draining to Chesapeake Bay. The URL is (2): http://onlinelibrary.wiley.com/doi/10.1111/j.1752-1688.2010.00482.x/full

The second is an application to nitrate data for 8 monitoring sites on the Mississippi River or its major tributaries (3). The URL is: http://pubs.acs.org/doi/abs/10.1021/es201221s

The manual available here assumes that the user understands the concepts underlying WRTDS. Thus, reading at least the first of these papers is necessary to understanding the manual. The method has been enhanced beyond what was published there. The enhancement is that it now properly handles censored data by using survival regression rather than ordinary regression. The details of that are in a manuscript currently in process by Doug Moyer and

Bob Hirsch.

This vignette will walk through the major functions provided by the EGRET package. The package dataRetrieval is required for importing data in a EGRET-friendly format. The dataRetrieval package, along with download and installation instructions can be found at: https://github.com/USGS-R/dataRetrieval

Installing dataRetrieval will provide a vignette similar to this document, with complete working examples of the main dataRetrieval functions.

The vignette is divided into four sections: EGRET Dataframes, Flow History, WRTDS Analysis, and WRTDS Results. This document assumes the reader is familiar with the dataRetrieval package. The examples will follow an analysis of nitrate on the Choptank River at Greensboro, MD. Further details can be found in the user guide that can be found on gitHub: https://github.com/USGS-R/EGRET/raw/Documentation/EGRET%2Bmanual_4.doc

2 EGRET Dataframes and Units

The EGRET package uses 3 default dataframes throughout the calculations, analysis, and graphing. These dataframes are Daily (2.1), Sample (2.2), and INFO (2.3). EGRET uses entirely SI units to store the data, but for purposes of output, it can report results in a wide variety of units, which will be discussed in (2.4). To start our exploration, the packages must be installed (check the appendix for detailed instructions (A)), then opened:

- > library(EGRET)
- > library(dataRetrieval)

2.1 Daily

The Daily dataframe initially is populated with the following columns by the dataRetrieval package.

After running the WRTDS calculations (as will be described in 5), the following columns are inserted into the Daily dataframe:

Table 1: Daily dataframe

ColumnName	Type	Description	Units
Date	Date	Date	date
Q	number	Discharge in cms	cms
Julian	number	Number of days since January 1, 1850	days
Month	integer	Month of the year [1-12]	months
Day	integer	Day of the year [1-366]	days
DecYear	number	Decimal year	years
MonthSeq	integer	Number of months since January 1, 1850	months
Qualifier	string	Qualifying code	character
i	integer	Index	days
LogQ	number	Natural logarithm of Q	numeric
Q7	number	7 day running average of Q	cms
Q30	number	30 running average of Q	cms

Table 2: Daily dataframe, post-WRTDS

ColumnName	Type	Description	Units
yHat	number	The WRTDS estimate of the log of concentration	numeric
SE	number	The WRTDS estimate of the standard error of yHat	numeric
ConcDay	number	The WRTDS estimate of concentration	$\mathrm{mg/L}$
FluxDay	number	The WRTDS estimate of flux	kg/day
FNConc	number	Flow normalized estimate of concentration	$\mathrm{mg/L}$
FNFlux	number	Flow Normalized estimate of flux	kg/day

2.2 Sample

The Sample dataframe initially is populated with the following columns by the dataRetrieval package.

After running the WRTDS calculations (as will be described in 5), the following columns are inserted into the Sample dataframe:

 $^{^1{\}rm Flow}$ columns are populated after calling the merge Report function.

Table 3: Sample dataframe

ColumnName	Type	Description	Units
Date	Date	Date	date
ConcLow	number	Lower limit of concentration	m mg/L
ConcHigh	number	Upper limit of concentration	$\mathrm{mg/L}$
Uncen	integer	Uncensored data (1=true, 0=false)	integer
ConcAve	number	Average concentration	mg/L
Julian	number	Number of days since January 1, 1850	days
Month	integer	Month of the year [1-12]	months
Day	integer	Day of the year [1-366]	days
DecYear	number	Decimal year	years
MonthSeq	integer	Number of months since January 1, 1850	months
SinDY	number	Sine of DecYear	numeric
CosDY	number	Cosine of DecYear	numeric
Q^{-1}	number	Discharge	cms
$-$ LogQ 1	number	Natural logarithm of flow	numeric

Table 4: Sample dataframe, post-WRTDS

ColumnName	Type	Description	Units
yHat	number	jack-knife estimate of the log of concentration	numeric
SE	number	jack-knife estimate of the standard error of yHat	numeric
ConcHat	number	jack-knife unbiased estimate of concentration	$\mathrm{mg/L}$

2.3 INFO

The INFO dataframe is used to store information about the measurements, such as station name, parameter name, drainage area, etc. There can be many additional, optional columns, but the following are required to initiate the EGRET analysis:

Table 5: INFO dataframe

ColumnName	Type	Description
shortName	string	Name of site, suitable for use in graphical headings
$\operatorname{staAbbrev}$	string	Abbreviation for station name, used in saveResults
paramShortName	string	Name of constituent, suitable for use in graphical headings
constit Abbrev	string	Abbreviation for constituent name, used in saveResults
drainSqKm	numeric	Drainage area in km ²
paStart ²	integer $(1-12)$	Starting month of period of analysis
paLong ²	integer (1-12)	Length of period of analysis in months

²paStart and paLong can be inserted using the setPA function

After running the WRTDS calculations (as will be described in 5), the following columns are automatically inserted into the INFO dataframe (the values will be discussed further sections):

Table 6: INFO dataframe, post-WRTDS

ColumnName	Description	Units
$\overline{\mathrm{bottomLogQ}}$	Lowest discharge in prediction surfaces	numeric
stepLogQ	Step size in discharge in prediction surfaces	numeric
nVectorLogQ	Number of steps in discharge, prediction surfaces	numeric
bottomYear	Starting year in prediction surfaces	numeric
stepYear	Step size in years in prediction surfaces	numeric
nVectorYear	Number of steps in years in prediction surfaces	$\operatorname{numeric}$
windowY	Half-window width in the time dimension	years
windowQ	Half-window width in the log discharge dimension	numeric
windowS	Half-window width in the seasonal dimension	years
$\min NumObs$	Minimum number of observations for regression	integer
$\min Num Uncen$	Minimum number of uncensored observations	integer

2.4 Units

EGRET uses entirely SI units to store the data, but for purposes of output, it can report results in a wide variety of units. The default is that concentration is measured in mg/L, discharge is cubic meters per second (cms), flux is kg/day, and drainage area is km^2. When discharge values are imported from USGS web services (using the dataRetrieval package), they are automatically converted from cubic feet per second (cfs) to cms unless the argument convet is set to FALSE. This can cause confusion if not careful.

Although the data is stored in the dataframes in SI, it is possible to report the results in a variety of units. For all functions that provide output, there are two arguments that can be defined to set the output units: qUnit and FluxUnit. qUnit and FluxUnit can be defined by a numeric code or name. There are two functions that can be called to see the options for qUnit and FluxUnit: printqUnitCheatSheet and printFluxUnitCheatSheet.

> printqUnitCheatSheet()

```
The following codes apply to the qUnit list:

1 = cfs (Cubic Feet per Second)

2 = cms (Cubic Meters per Second)

3 = thousandCfs (Thousand Cubic Feet per Second)

4 = thousandCms (Thousand Cubic Meters per Second)

5 = mmDay (mm per day)

6 = mmYear (mm per year)
```

When a function has an input argument qUnit, you can define the flow units with the index (1-6) as shown above. The choice should be based on the units that are customary for the audience, but also so that the discharge values don't have too many digits to the right or left of the decimal point.

> printFluxUnitCheatSheet()

```
The following codes apply to the fluxUnit list:

1 = poundsDay ( pounds/day )

2 = tonsDay ( tons/day )

3 = kgDay ( kg/day )

4 = thousandKgDay ( thousands of kg/day )

5 = tonsYear ( tons/year )

6 = thousandTonsYear ( thousands of tons/year )

7 = millionTonsYear ( millions of tons/year )

8 = thousandKgYear ( thousands of kg/year )

9 = millionKgYear ( millions of kg/year )

10 = billionKgYear ( billions of kg/year )

11 = thousandTonsDay ( thousands of tons/day )

12 = millionKgDay ( millions of kg/day )
```

When a function has an input argument FluxUnit, you can define the flux units with the index (1-12) as shown above. The choice should be based on the units that are customary for the audience, but also so that the flux values don't have too many digits to the right or left of the decimal point.

3 Flow History

This section describes functions included in the EGRET package that provide a variety of table and graphical outputs looking only at flow statistics based on time-series smoothing. These functions were designed for studies of long-term streamflow change and work best for daily streamflow data sets of 50 years or longer. This type of analysis might be useful for studying

At this point it is assumed that you have loaded the daily discharge record and created the Daily data frame, and also entered the required meta-data into the INFO data frame. We will walk through an example from the Rio Grande gaging station in Embodo, NM. This is the first stream gage station in the USGS, established by John Wesley Powell in 1888.

```
> #Rio Grande at Embudo, NM
> siteID <- "08279500"
> startDate <- ""
> endDate <- ""</pre>
```

- > Daily <- getDVData(siteID, "00060", startDate, endDate, interactive=FALSE)
- > INFO <- getMetaData(siteID,"",interactive=FALSE)</pre>
- > INFO\$shortName <- "Rio Grande at Embudo, NM"

The first choice you need to make is what 'period of analysis' to use (pa). What is the period of analysis? If we want to examine our data set as a time series of water years, then the period of analysis is the water year. If we want to examine the data set as calendar years then the period of analysis should be the calendar year. We might want to examine the winter season, which we might want to define as December, January and February, then those 3 months become the period of analysis. We might even want to examine September only then September becomes the period of analysis. The only constraints on the definition of a period of analysis are these: It must be defined in terms of whole months. It must be a set of contiguous months (like March-April-May). And it must have a length that is no less than 1 month and no more than 12 months. It can be uniquely defined by two arguments: paLong and paStart. paLong is the length of the period of analysis, and paStart is the first month of the period of analysis. The following examples summarize paLong and paStart.

Table 7: Period of Analysis Information

PeriodOfAnalysis	paStart	PaLong
Calendar Year	1	12
Water Year	10	12
Winter	12	3
September	9	1

To set a period running from December through February:

> INFO <- setPA(paStart=12,paLong=3)

To set the default value (water year):

> INFO <- setPA()

The next step is to create the annual series of flow statistics. These will be stored in a matrix called annual Series that contain the following statistics:

To create the annual Series matrix, using the function make Annual Series:

> annualSeries <- makeAnnualSeries()</pre>

Once the annual Series matrix is created, the plots of any of the stored statistics can be generated with the plotFlowSingle function.

Table 8: Index of Statistics Information

istat	Name
1	1-day minimum flow
2	7-day minimum flow
3	30-day minimum flow
4	median flow
5	mean flow
6	30-day maximum flow
7	7-day maximum flow
8	1-day maximum flow

3.1 Plotting Options

There are several plotting options available for studying flow history once the annual Series has been created.

3.1.1 plotFlowSingle

The simplest way to look at these time series is with the function plotFlowSingle. The statistic index (istat) must be defined, but other input arguements can defined. To see a list of these optional arguments and other information about the function, type ?plotFlowSingle in the R console. In this example, we can plot the 7-day maximum over the water year in thousands of cfs (Figure 1):

- > # plotFlowSingle(istat=5,qUnit=3)
- > #identical to:
- > plotFlowSingle(istat=7,qUnit="thousandCfs")

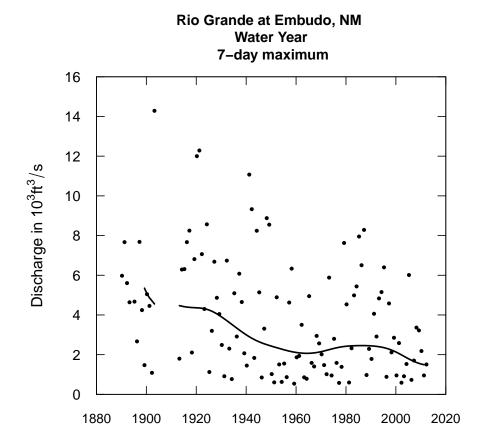


Figure 1: 7-day Maxiumum Flow (istat=7)

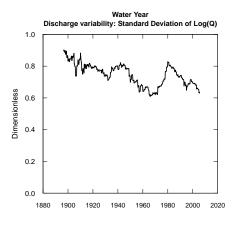
3.1.2 plotSDLogQ

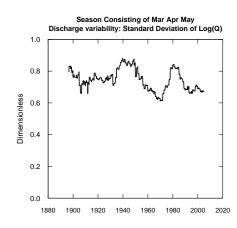
This function produces a graphic of the running standard deviation of the log of daily discharge over time. The idea is to get some idea of how variability of daily discharge is changing over time. By using the standard deviation of the log discharge the statistic becomes dimensionless. It also means that it is a way of looking at variability quite aside from average values, so, in the case of a system where discharge might be increasing over a period of years, this provides a way of looking at the variability relative to that changing mean value. It is much like a coefficient of variation, but it has sample properties that make it a smoother measure of variability. There are often comments about how things like urbanization or enhanced greenhouse gases in the atmosphere are bringing about an increase in variability, this is one way to explore that idea. In the simplest case the call is (Figure 2a):

- > INFO <- setPA()
- > plotSDLogQ()

If you were just interested in the variability in spring (March-April-May), you could change paStart and paLong using the setPA function (Figure 2b). These figures show there is little change in variability on the Rio Grande between the water year and spring.

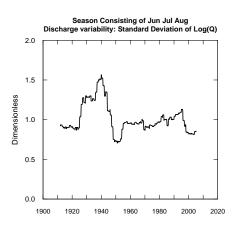
> INFO <- setPA(paStart=3, paLong=3)
> plotSDLogQ()

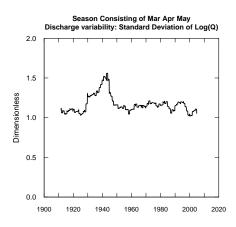




(a) Water Year (b) Spring (March-May) Figure 2: Discharge variability on the Rio Grande

A more interesting comparison might be between spring and summer on the Red River of the North (Figure 3). This figure shows that there is generally more variability in discharge in the spring compared to the summer.





(a) Summer (June-August) (b) Spring (March-May) Figure 3: Discharge variability on the Red River of the North, ND

3.1.3 plotQTimeDaily

plotQTimeDaily is simply a time series plot of discharge. But, it is most suited for showing events above some discharge threshold. In the simplest case, it can plot the entire record, but given the line weight and use of an arithmetic scale it will primarily provide a visual focus on the higher values. plotQTimeDaily requires startYear and endYear, along with some other optional arguements (see ?plotQTimeDaily for more details).

Returning to our example concerning the Rio Grande (Figure 4):

> plotQTimeDaily(1990,2000,qLower=2,qUnit=3)

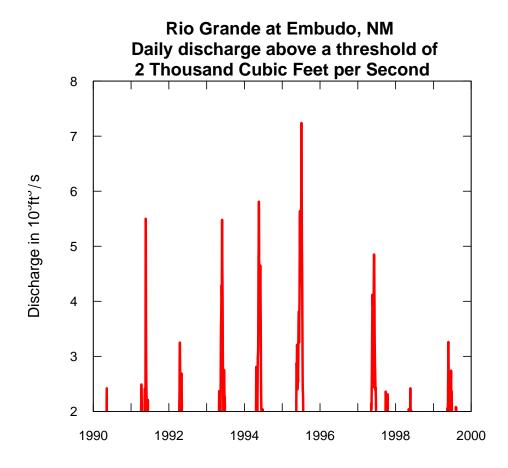


Figure 4: Discharge above a threshold

3.1.4 plotFour

- > annualSeries <- makeAnnualSeries()</pre>
- > plotFour(qUnit=3)

Rio Grande at Embudo, NM Season Consisting of Mar Apr May

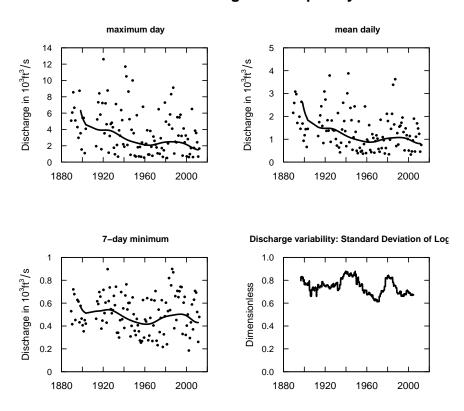


Figure 5: Default plotFour

${\bf 3.1.5} \quad {\bf plotFourStats}$

> plotFourStats(qUnit=3)

Rio Grande at Embudo, NM Season Consisting of Mar Apr May

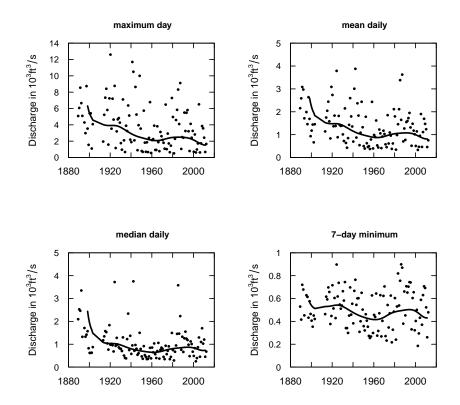


Figure 6: Default plotFourStats

3.2 Table Options

Rathar than graphically, it is sometimes easier to consider the results in table formats.

3.2.1 printSeries

Similar to the function plotFlowSingle, the printSeries will print the requested flow statistics (Table 8). A small sample of the output is printed below.

> printSeries(istat=3, qUnit=3)

Rio Grande at Embudo, NM Water Year 30-day minimum

Thousand		${\tt Cubic}$	Feet	per	Second
year	anı	nual	smoot	thed	
	va	alue	value		
1899	0	. 280	0.29	96	
1900	0	. 208	0.28	35	
1901	0	. 169	0.27	77	
1902	0	.320	0.27	72	
2011	0	. 252	0.24	1 8	
2012	0	. 257	1	ΝA	

3.2.2 tableFlowChange

Another way to look at the results is to consider how much the smoothed values change between various pairs of years. These changes can be represented in four different ways.

- As a change between the first and last year of the pair, expressed in the flow units selected.
- As a change between the first and last year of the pair, expressed as a percentage of the value in the first year
- As a slope between the first and last year of the pair, expressed in terms of the flow units per year.
- As a slope between the first and last year of the pair, expressed as a percentage change per year (a percentage based on the value in the first year).

There is another argument that can be very useful in this function: yearPoints. In the default case, the set of years that are compared are at 5 year intervals along the whole data set. If the data set was quite long this can be a daunting number of comparisons. For example, in an 80 year record, there would be 136 such pairs. Instead, we could look at changes for every 20 years starting in 1930:

> tableFlowChange(istat=3, qUnit=3, yearPoints=c(1930, 1950, 1970, 1990, 2010))

Rio Grande at Embudo, NM Season Consisting of Mar Apr May 30-day minimum

Streamflow Trends

time sp	an	change	slope	change	slope
		10^3 cfs 1	l0^3 cfs /yr	%	%/yr
1930 to	1950	-0.089	-0.0045	-16	-0.8

1930	to	1970	-0.1	-0.0025	-18	-0.45
1930	to	1990	-0.046	-0.00077	-8.3	-0.14
1930	to	2010	-0.11	-0.0013	-19	-0.24
1950	to	1970	-0.011	-0.00054	-2.3	-0.12
1950	to	1990	0.043	0.0011	9.2	0.23
1950	to	2010	-0.016	-0.00026	-3.4	-0.056
1970	to	1990	0.054	0.0027	12	0.59
1970	to	2010	-0.0049	-0.00012	-1.1	-0.027
1990	to	2010	-0.059	-0.0029	-12	-0.58

4 Water Quality Analysis (pre-WRTDS)

Before running the WRTDS model, it is very helpful to take a look at the measured data in a graphical way to understand its behavior and to identify things that might be errors in the data set or learn about the temporal distribution of the data (identify gaps) prior to running the model. It is always best to clear up these issues before moving forward.

In this section and the next, we will use the Choptank River at Greensboro, MD as our example case. The Choptank River is a major tributary of the Chesapeake Bay. Inorganic nitrogen (nitrate and nitrite) has been measured from 1979. First, we need to get the streamflow and nitrate data into R, then use the mergeReport function to associate flow with the discrete measured water quality data.

```
> siteID <- "01491000" #Choptank River at Greensboro, MD
> startDate <- "1979-10-01"
> endDate <- "2011-09-30"
> param<-"00631"
> INFO<- getMetaData(siteID,param,interactive=FALSE)
> INFO$shortName <- "Choptank River"
> Sample <- getSampleData(siteID,param,startDate,endDate)
> Sample <- mergeReport()</pre>
```

4.1 Water Quality Plotting Variables

The next section will cover the available plots in the EGRET package. This section will briefly summarize common input variables (arguments) for those functions.

Table 9: Variables used in water quality analysis plots

Argument	Table 9: Variables used in water quality analysis plots Definition			
qUnit	Determines what units will be used for discharge, see 2.4			
printTitle	If TRUE the plot has a title. If FALSE no title (useful for publications where			
1	there will be a caption)			
qLower	The lower bound on the discharge on the day of sampling that will be used in			
-	forming a subset of the sample data set that will be displayed in the graph. It			
	is expressed in the units specified in qUnit. If qLower = NA, then the lower			
	bound is set to zero.			
qUpper	The upper bound on the discharge on the day of sampling that will be used in			
	forming a subset of the sample data set that will be displayed in the graph. It			
	is expressed in the units specified in qUnit. If qUpper = NA, then the lower			
	bound is set to infinity.			
paLong	The length of the time period that will be used in forming a subset of the			
	sample data set that will be displayed in the graph, expressed in months.			
paStart	The starting month for the time period that will be used in forming a subset			
	of the sample data set that will be displayed in the graph. It is expressed in			
	months (calendar months).			
concMax	The upper limit on the vertical axis of graphs showing concentration values			
	in mg/L (NA sets value to just above maximum).			
concMin	The lower limit on the vertical axis of graphs showing concentration values in			
	mg/L (NA sets value to just below minimum for log scales, zero for linear).			
fluxUnit	Determines what units will be used for flux (see Section 2.4).			
fluxMax	The upper limit on the vertical axis of graphs showing flux values.			

4.2 Water Quality Plots

5 WRTDS Analysis

Weighted Regressions on Time, Discharge and Season (WRTDS) creates a model of long-term trends in river-water quality, seasonal components, and discharge-related components of the behavior of measured water-quality parameters. In this section, we will step though the process require for a WRTDS analysis. The following section (6) will detail the available methods to view and evaluate the model results.

- > modelEstimation()
- > AnnualResults<-setupYears()

6 WRTDS Results

A Appendix 1: Getting Started

This section describes the options for downloading and installing the dataRetrieval package.

A.1 New to R?

If you are new to R, you will need to first install the latest version of R, which can be found here: http://www.r-project.org/.

There are many options for running and editing R code, one nice environment to learn R is RStudio. RStudio can be downloaded here: http://rstudio.org/. Once R and RStudio are installed, the environment package needs to be installed as described in the next section.

At any time, you can get information about any function in R by typing a question mark before the functions name. This will open a file (in RStudio, in the Help window) that describes the function, the required arguments, and provides working examples.

> ?getJulian

To see the raw code for a particular code, type the name of the function:

```
> getJulian
```

```
function(date) {
    # enter date in quotes for example "1949-09-30"
    # program returns the julian date
    dateTime <- as.Date(date)
    Julian <- as.numeric(julian(dateTime, origin = as.Date("1850-01-01")))
    return(Julian)
}
<environment: namespace:EGRET>
```

A.2 R User: Installing EGRET

To install the EGRET packages and it's dependencies:

It is a good idea to re-start the R enviornment after installing the package, especially if installing an updated version (that is, restart RStudio). Some users have found it necessary to delete the previous version's package folder before installing newer version of EGRET. If you are experiencing issues after updating a package, trying deleting the package folder - the default location for Windows is something like this: C:/Users/userA/Documents/R/winlibrary/2.15/EGRET, and the default for a Mac: /Users/userA/Library/R/2.15/library/EGRET. Then, re-install the package using the directions above. Moving to CRAN should solve this problem.

After installing the package, you need to open the library each time you re-start R. This is done with the simple command:

```
> library(dataRetrieval)
```

> library(EGRET)

Using RStudio, you could alternatively click on the checkbox for dataRetrieval and EGRET in the Packages window.

A.3 R Developers: Installing EGRET from gitHub

Alternatively, R-developers can install the most recent (not-necessarily stable) version of EGRET directly from gitHub using the devtools package. devtools is available on CRAN. Simply type the following commands into R to install the latest version of EGRET available on gitHub. Rtools (for Windows) and appropriate LATEX tools are required. Be aware that the version installed using this method isn't necessarily the same as the version in the stable release branch.

```
> library(devtools)
> install_github("dataRetrieval", "USGS-R")
> install_github("EGRET", "USGS-R")
```

To then open the library, simply type:

```
> library(dataRetrieval)
> library(EGRET)
```

References

[1] Helsel, D.R. and R. M. Hirsch, 2002. Statistical Methods in Water Resources Techniques of Water Resources Investigations, Book 4, chapter A3. U.S. Geological Survey. 522 pages. http://pubs.usgs.gov/twri/twri4a3/

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- [3] Sprague, L. A., Hirsch, R. M., and Aulenbach, B. T. (2011), Nitrate in the Mississippi River and Its Tributaries, 1980 to 2008: Are We Making Progress? Environmental Science & Technology, 45 (17): 7209-7216. doi: 10.1021/es201221s http://pubs.acs.org/doi/abs/10.1021/es201221s