Trend Analysis of Uncensored Major Ions

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Abstract

This example illustrates the data manipulations for the seasonal Kendall analysis of uncensored data. Major ions are typically uncensored in natural waters and provide a useful example. This example also uses a common time frame for all of the trend tests. The common time frame facilitates comparing trends among the stations. Most often users will want to divide trend analyses into similar groups of analytes like major ions, nutrients and so forth because they will be analyzed in similar ways and will have common sampling time frames.

Contents

1 Introduction

The data used in this application are a small subset of the data used by Schertz and others (1991). The data are samples taken from water year 1969 (October, 1968) through water year 1989 (September, 1989). Nineteen stations were selected and only calcium and chloride were selected for the major ions. The data were modified by removing the remark columns associated with those constituents to make the analysis more straightforward.

```
> # Load the restrend and smwrBase packages and the data
> library(restrend)
> library(smwrBase)
> data(EstrendSub)
> head(EstrendSub)

     STAID      DATES    QI QD RN.organic PN.organic RAmmonia
1 07227500 1968-10-01   7.6 NA                    NA
2 07227500 1968-10-03   5.3 NA                    NA
3 07227500 1968-10-16 532.0 NA                    NA
4 07227500 1968-10-19  17.0 NA                    NA
5 07227500 1968-11-01  17.0 NA                    NA
6 07227500 1968-12-01   6.6 NA                    NA
  PAmmonia RKjeldahl PKjeldahl RTotal.P PTotal.P RCopper PCopper
1       NA                  NA                NA              NA
2       NA                  NA                NA              NA
3       NA                  NA                NA              NA
4       NA                  NA                NA              NA
5       NA                  NA                NA              NA
6       NA                  NA                NA              NA
  RIron PIron Calcium Chloride
1          NA      95      280
2          NA      NA       NA
3          NA      42      106
4          NA     121      435
5          NA     150      512
6          NA     138      510
```

2 Summarize the Sample Data

In general, it is desirable, but not necessary, to subset the data before proceeding with the analysis of a subset of the constituents. Before these data are subsetted, the FLOW column must be created. The flow data are in two columns `QI`, the flow at the time of the sample; and `QD`, the mean flow on the day of the sample. The `coalesce` function in the `smwrBase` package can used to select the non-missing value for flow.

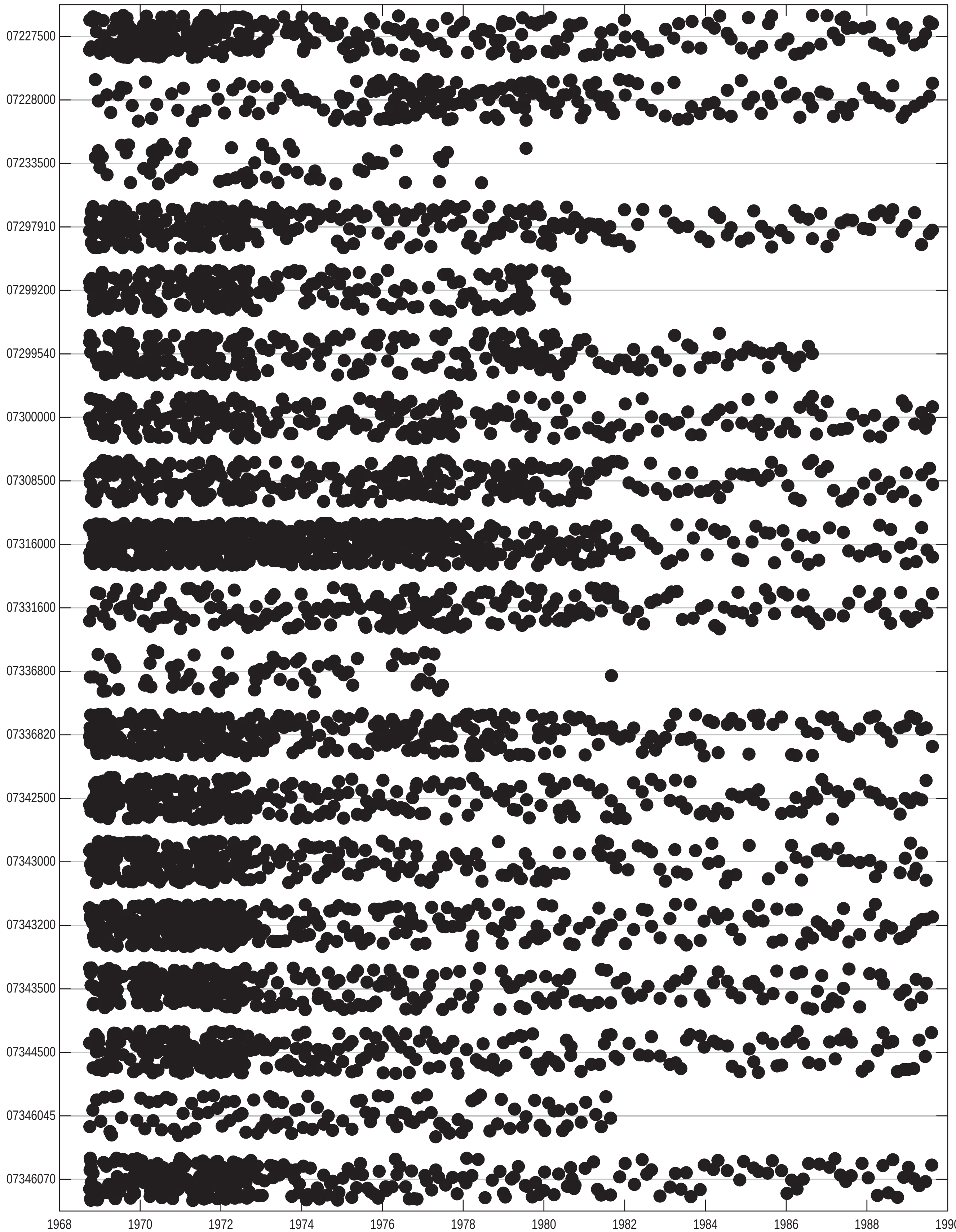
```
> # Compute FLOW, the coalesce function is in smwrBase
> EstrendSub <- transform(EstrendSub, FLOW=coalesce(QI, QD))
> # Create the subset
> Majors <- subset(EstrendSub, select=c("STAID", "DATES", "FLOW",
+     "Calcium", "Chloride"))
```

The `sampReport` function creates a simple PDF file that contains a report of the sample date ranges and graph of samples for each site. It can be used to help define the starting and ending date ranges for the trend tests as well as identifying sample gaps and other sampling issues.

```
> # Create the report
> sampReport(Majors, DATES="DATES", STAID="STAID", file="MajorIonSampling")
```

The call to `sampReport` returns the file name invisibly (MajorIonSampling.pdf). Because it is a full-size portrait PDF file, it is inserted here with compressed pages. The report gives the actual begin and end dates for sampling and the graph shows the sampling dates for each station. It is easy to see that 5 stations (07233500, 07299200, 07299540, 07336800, and 07346045) were not sampled for the entire retrieval period.

	STAID	FirstSamp	LastSamp	NumSamp
1	07227500	1968−10−01	1989−08−15	350
2	07228000	1968−11−21	1989−08−16	198
3	07233500	1968−11−21	1979−07−24	62
4	07297910	1968−10−01	1989−08−15	308
5	07299200	1968−10−01	1980−07−09	217
6	07299540	1968−10−01	1986−08−25	276
7	07300000	1968−10−01	1989−08−16	283
8	07308500	1968−10−01	1989−08−18	336
9	07316000	1968−10−01	1989−08−16	694
10	07331600	1968−10−01	1989−08−15	228
11	07336800	1968−10−07	1981−09−03	69
12	07336820	1968−10−01	1989−08−15	393
13	07342500	1968−10−01	1989−06−19	325
14	07343000	1968−10−01	1989−06−19	317
15	07343200	1968−10−01	1989−08−16	366
16	07343500	1968−10−01	1989−06−21	303
17	07344500	1968−10−01	1989−08−07	294
18	07346045	1968−10−03	1981−08−27	109
19	07346070	1968−10−01	1989−08−10	300


07227500
07228000
07233500
07297910
07299200
07299540
07300000
07308500
07316000
07331600
07336800
07336820
07342500
07343000
07343200
07343500
07344500
07346045
07346070
1968
1970
1972
1974
1976
1978
1980
1982
1984
1986
1988
1990

3 Set up the Project

The user must balance the need to include as many stations as possible and the targeted time frame for the trend estimation. For these data, 5 stations have incomplete record, but to include all of those stations, the analysis period would need to be much shorter, though water year 1978. This example will use the full retrieval period.

The (setProj) function sets up the trend estimation project. There are many arguments to (setProj), see the documentation for details. The constituent names or response variable names are referred to as `Snames` in keeping with the names used in the original ESTREND.

After projects have been set up, the user can get a list of the projects by using `lsProj` or can specify a project to use with `useProj`. The function `useProj` must be used to continue working on a project after the user quits from the R session.

```
> # Set up the project
> setProj("majors", Majors, STAID="STAID", DATES="DATES",
+         Snames=c("Calcium", "Chloride"), FLOW="FLOW",
+         type="seasonal", Start="1968-10-01", End="1989-10-01")

[1] "majors"
```

The (setProj) function creates a folder in the users workspace with that name. That folder contains `R` data that are updated after each successful call to an analysis function in `restrend`. Table 1 describes the data created in this example's call to (setProj). Any object of class "matrix" or "by" are indexed by station and sname.

Table 1. The data created by (setProj).

Name	Class	Description
estrend.cl	list	A record of the calls to analysis functions.
estrend.cn	matrix	A description of the censoring. May be "none," "left," or "multiple."
estrend.cp	matrix	The percent of observations that are left-censored.
estrend.df	by	The dataset, contains STAID, DATES, FLOW, and the response variable.
estrend.in	list	Information about the project, such as the start and end dates and the names of columns in each dataset.
estrend.sl	by	Details from the seasonal selection process. Each is a list from the potential comparisons from 12, 6, 4, and 3 seasons per year definition. See Lorenz (2014) for details.
estrend.ss	matrix	The "best" seasonal definition from the analysis recorded in `estrend.sl`.
estrend.st	matrix	The status for each station and sname. Must be "OK" to continue with the trend analysis.

It is useful to verify which stations and snames will be analyzed and what the seasonal definitions are. The user need only enter the name of the R data object in the console. For these data, the seasonal definition is 0 in all cases where the status is not "OK."

```
> # Which are OK?
> estrend.st
```

```
          snames
stations   Calcium        Chloride      
  07227500 "OK"           "OK"          
  07228000 "OK"           "OK"          
  07233500 "short record" "short record"
  07297910 "OK"           "OK"          
  07299200 "short record" "short record"
  07299540 "short record" "short record"
  07300000 "OK"           "OK"          
  07308500 "OK"           "OK"          
  07316000 "OK"           "OK"          
  07331600 "OK"           "OK"          
  07336800 "short record" "short record"
  07336820 "OK"           "OK"          
  07342500 "OK"           "OK"          
  07343000 "OK"           "OK"          
  07343200 "OK"           "OK"          
  07343500 "OK"           "OK"          
  07344500 "OK"           "OK"          
  07346045 "short record" "short record"
  07346070 "OK"           "OK"          

> # What seasonal definition?
> estrend.ss

          snames
stations   Calcium Chloride
  07227500       6        6
  07228000       6        6
  07233500       0        0
  07297910       6        6
  07299200       0        0
  07299540       0        0
  07300000       6        6
  07308500       6        6
  07316000      12       12
  07331600      12       12
  07336800       0        0
  07336820      12       12
  07342500      12       12
  07343000      12       12
  07343200      12       12
  07343500      12       12
  07344500      12       12
  07346045       0        0
  07346070      12       12
```

4 Flow Adjustment

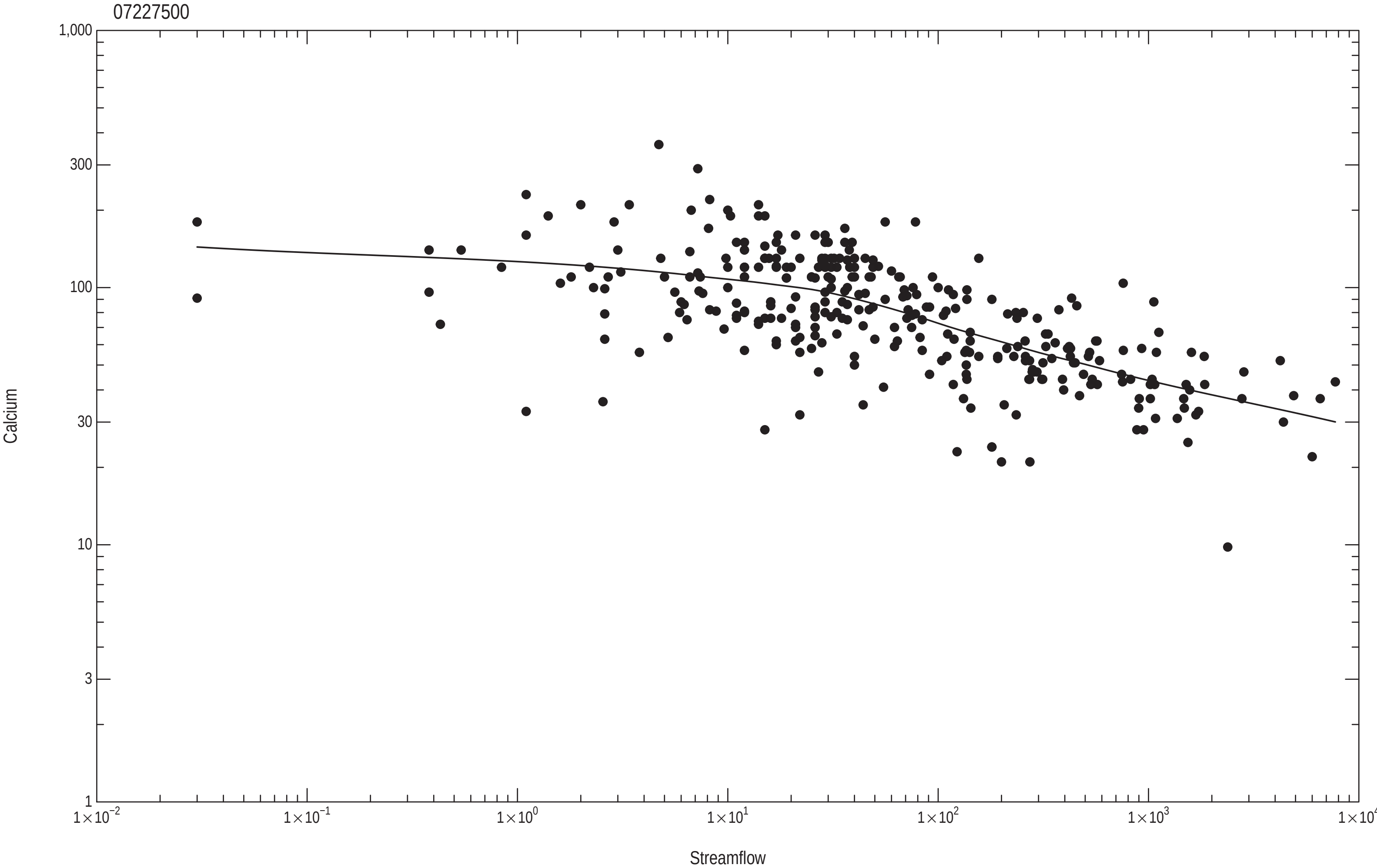
Computing flow-adjusted concentrations (flow adjustment) is an optional step in seasonal Kendall trend analysis. It is only appropriate for uncensored or slightly censored data. If the data are censored, the censoring is ignored and the values are taken as the detection limit. Flow adjustment is performed using the `flowAdjust` function and can immediately follow the call to `setProj`.

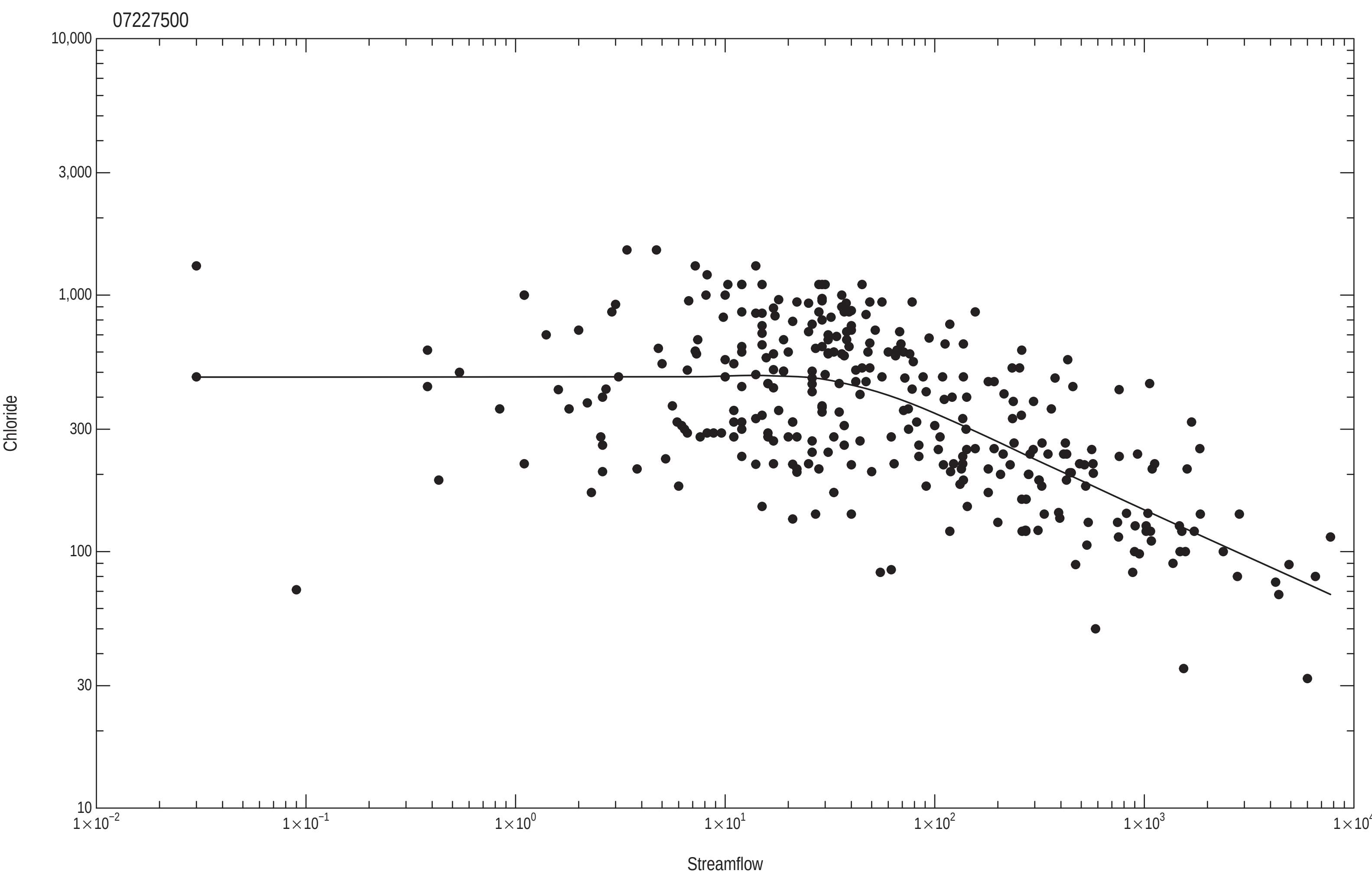
By default, all stations and snames are flow adjusted by `flowAdjust`. But specific combinations can be separately adjusted, using a different span for the LOWESS procedure for example, or if no satisfactory fit can be found, selected combinations can be completely undone by the `undoFA` function. Note that no relation between flow and concentration is not necessarily an unsatisfactory fit.

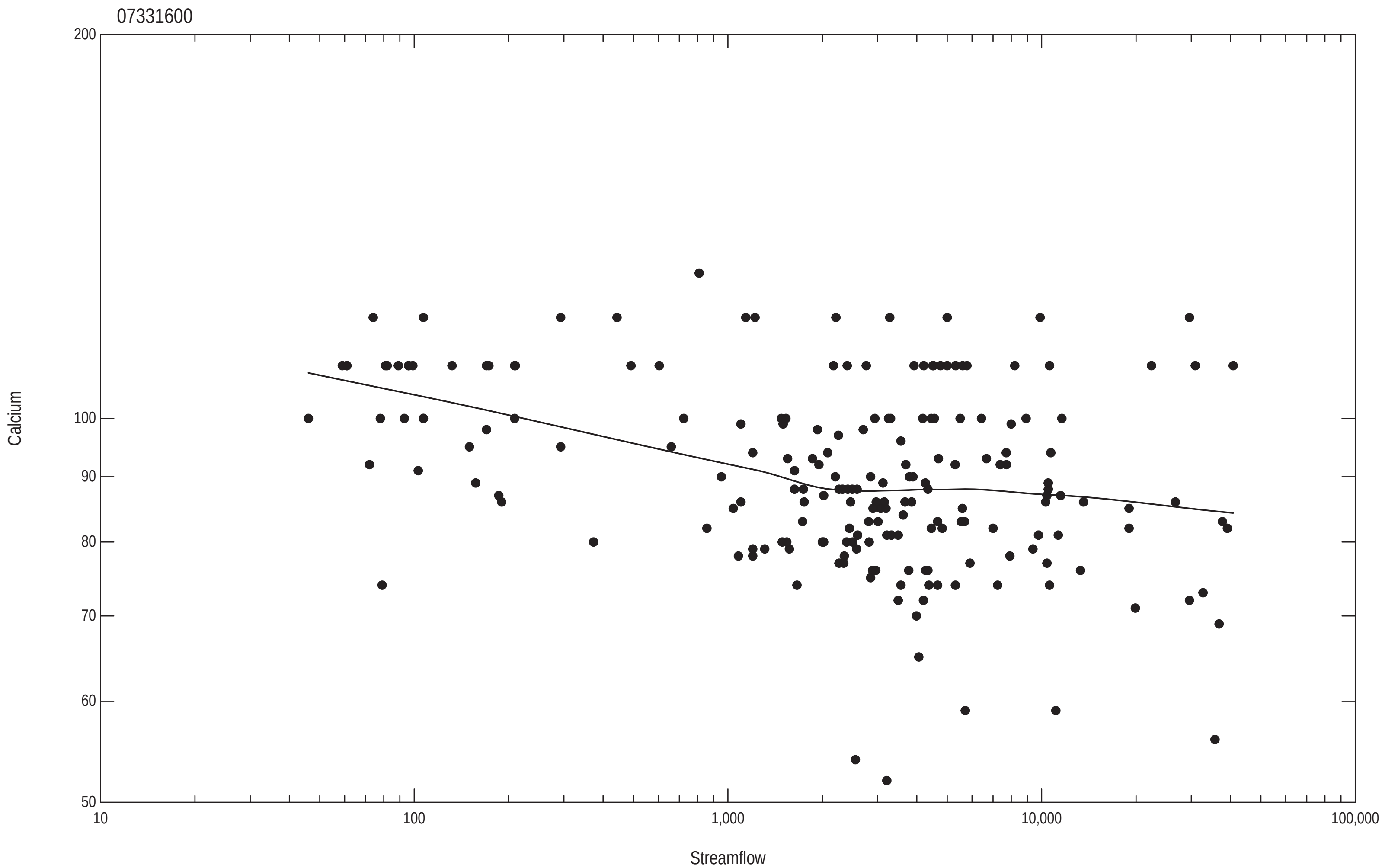
The `flowAdjust` function creates a PDF report, and returns the name of the report. The report shows graphs of flow and concentration by station on each page. Up to 6 combinations are shown on a page. For any seasonal Kendall trend test with flow adjustment, the user should review all flow-concentration relation. Only 2 pages are shown in this example, the first illustrates an acceptable fit and the second a marginal fit. The user may choose to revise other flow adjustments or accept all flow adjustments, but those for station 07331600 were selected to demonstrate customized flow adjustment.

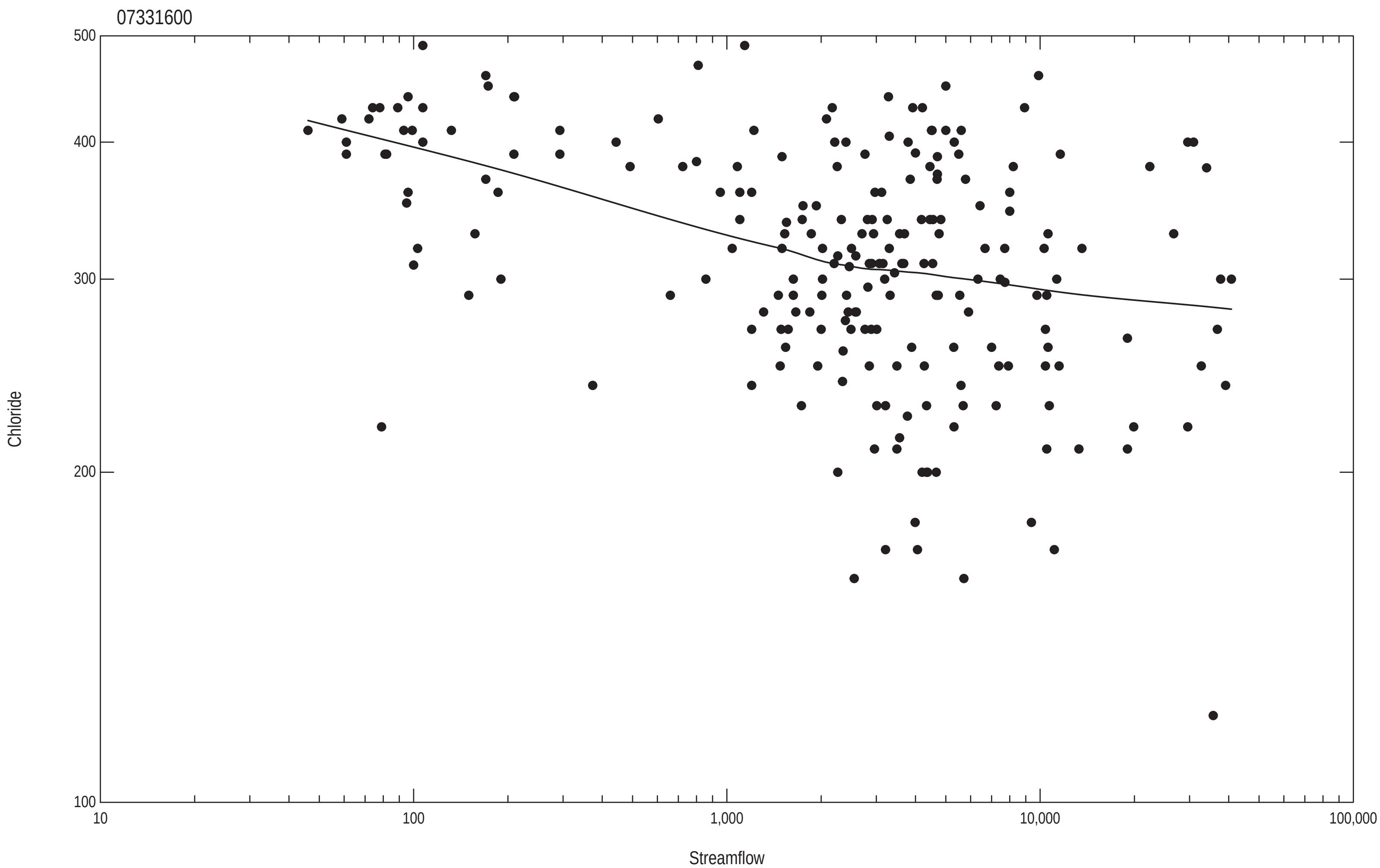
```
> # Do the flow adjustment accepting all defaults
> flowAdjust()
```

```
[1] "majors_fa.pdf"
```


07227500
Calcium
1,000
300
100
30
10
3
1
Streamflow
1×10⁻²
1×10⁻¹
1×10⁰
1×10¹
1×10²
1×10³
1×10⁴


07227500
Chloride
10,000
3,000
1,000
300
100
30
10
Streamflow
1×10⁻²
1×10⁻¹
1×10⁰
1×10¹
1×10²
1×10³
1×10⁴

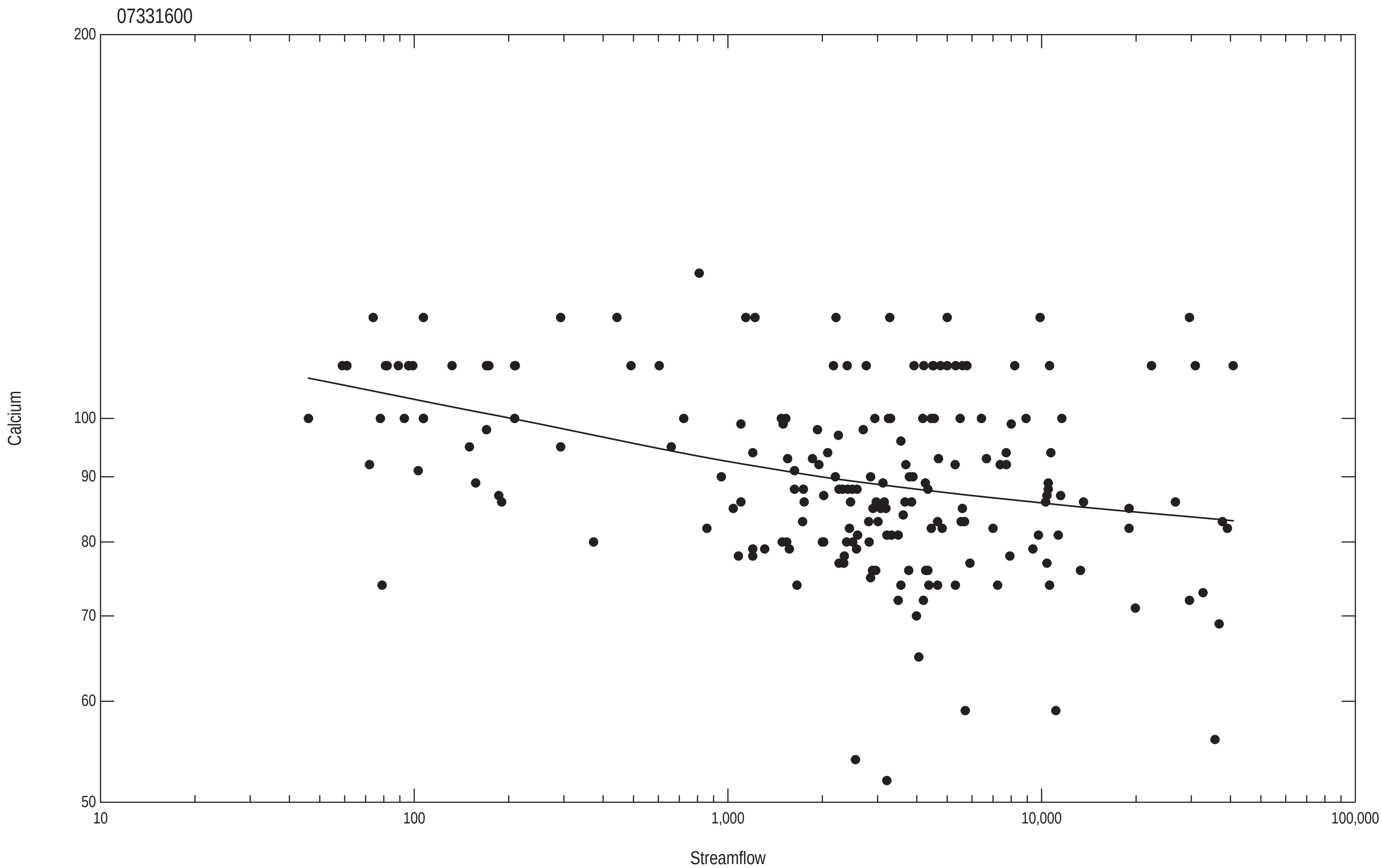

07331600
Calcium
200
100
90
80
70
60
50
10
100
1,000
10,000
100,000
Streamflow

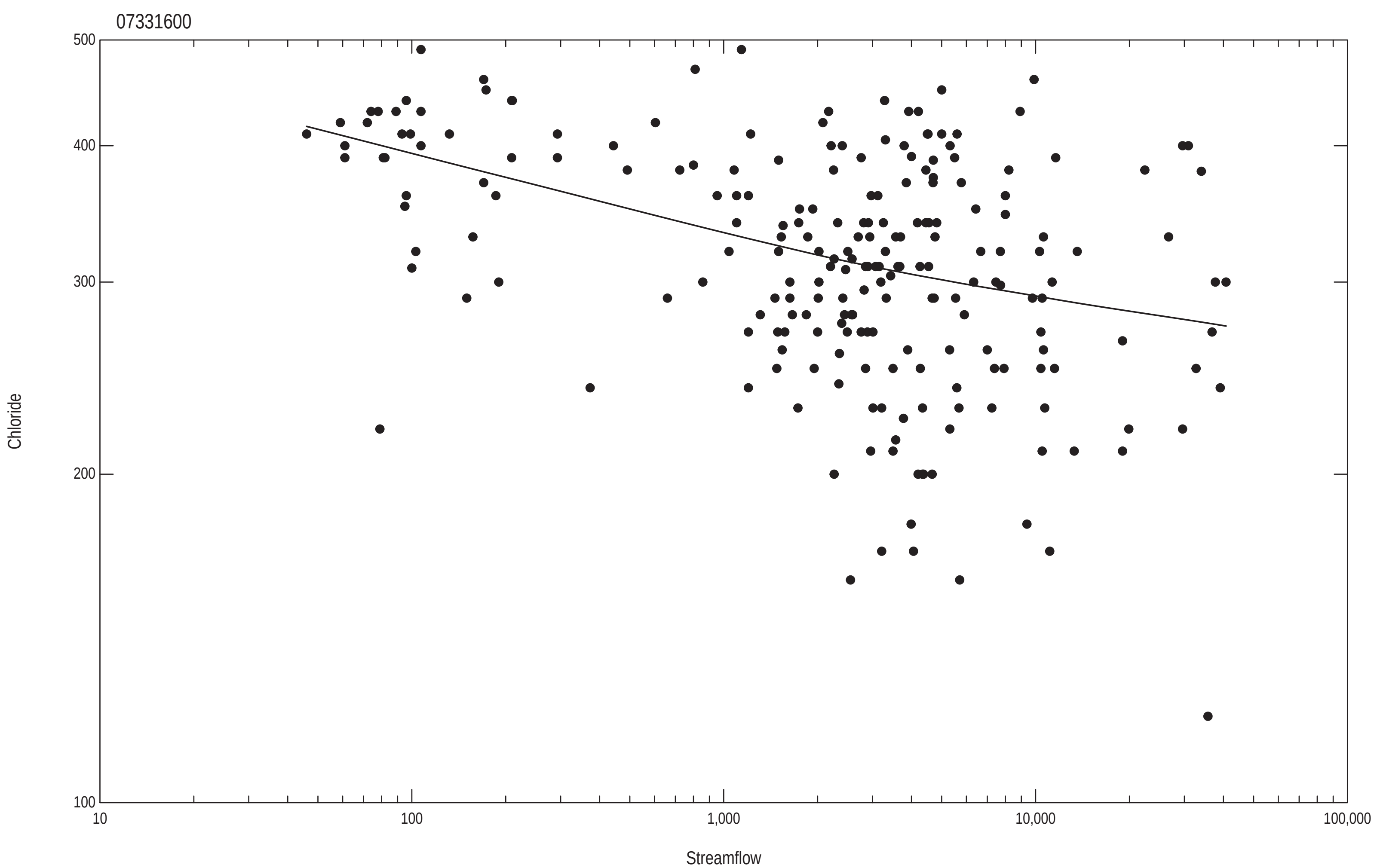

07331600
Chloride
500
400
300
200
100
10
100
1,000
10,000
100,000
Streamflow

The revised fit shows an improved, more smooth fit to the data.

```
> # Do the flow adjustment accepting all defaults
> flowAdjust(Station="07331600", Snames=c("Calcium", "Chloride"), span=1)

[1] "majors_fa_01.pdf"
```


07331600
Calcium
200
100
90
80
70
60
50
10
100
1,000
10,000
100,000
Streamflow


07331600
Chloride
500
400
300
200
100
10
100
1,000
10,000
100,000
Streamflow

5 Seasonal Kendall Trend Test

After the optional flow-adjustment, these data are ready for the seasonal Kendall trend test. The function `SKTrends` executes the trend test on all valid combinations of stations and snames. It can also execute the test on subsets if some changes need to be made. An important argument is `nseas`, which can be used to force all analyses to use the same seasonal definition. This is essential for the regional seasonal Kendall test and an important consideration for other regional assessments because it levels the playing field for determining significant trends.

The `SKTrends` function also creates a PDF file that contains the result of the analysis and a series graph on each page. See the documentation for `seriesPlot` for information about that graph. The file reports the results for each sname by station with the flow-adjusted results following the untransformed results. Most trends are very small for these data; only the reports for Calcium at 07228000 is shown.

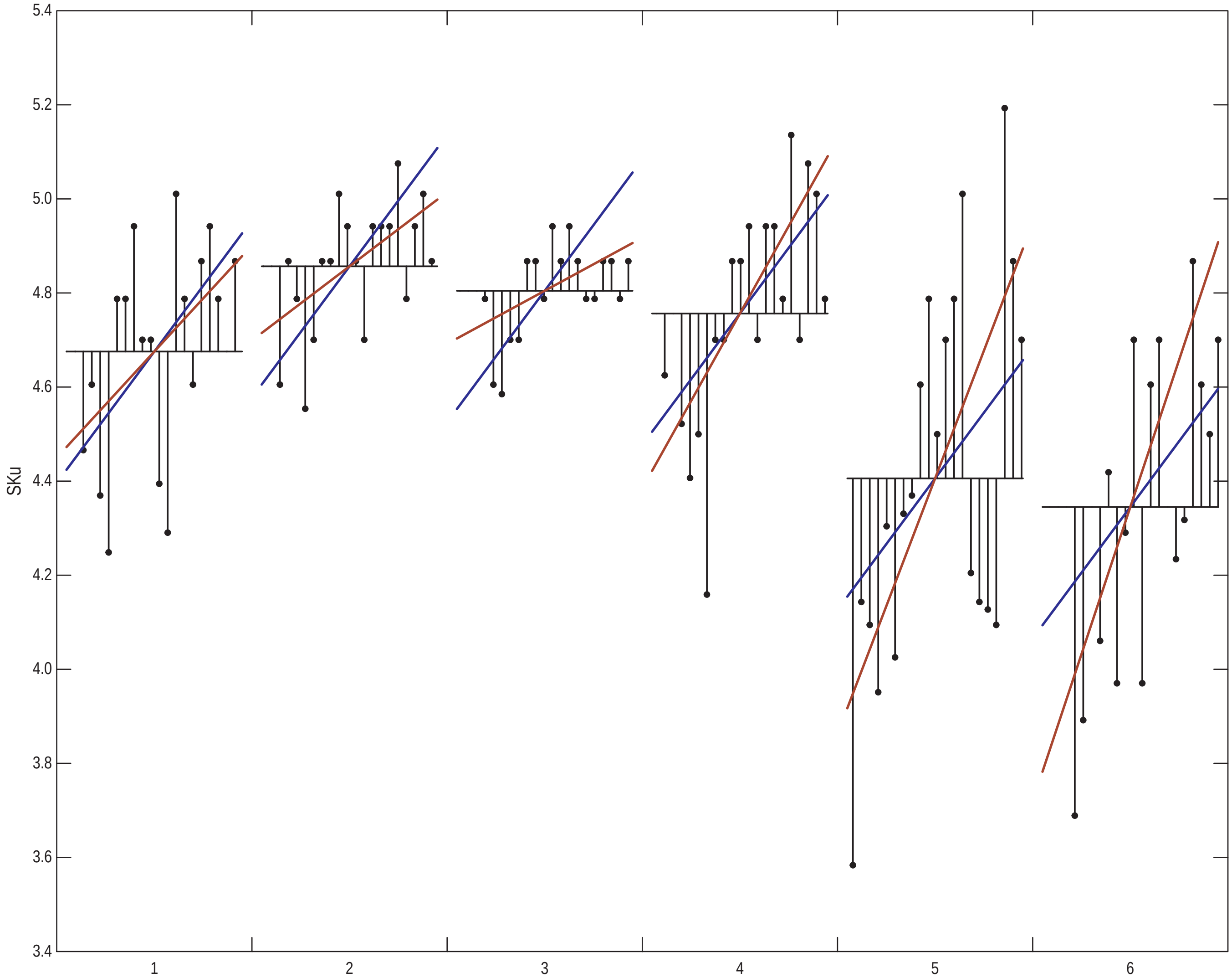
```
> # Trend tests, accepting default seasons
> SKTrends()
```

```
[1] "majors_sk.pdf"
```

```
07228000  Calcium

 Seasonal Kendall with correlation correction

data:  log(Calcium) (21 years and 6 seasons)
tau = 0.41513, p-value = 0.0003365
alternative hypothesis: true slope is not equal to 0
sample estimates:
      slope median.data median.time
 0.02154697  4.70048046 10.50000000
```



6 Trend Results

When completed, or to check on intermediate results, the estimated trends can be extracted using the `getTrends` function. By default, all stations and snames are extracted. The output dataset is explained in the documentation for `getTrends`. The user has the option to set a significance level to determine whether there is a significant trend, the default level is 0.05.

```
> # get the trends
> majors.tnd <- getTrends()
> print(majors.tnd)
```

```
    Station Response                           Type NumYears
1  07227500  Calcium    uncensored seasonal Kendall       21
2  07227500  Calcium flow-adjusted seasonal Kendall       21
3  07227500 Chloride    uncensored seasonal Kendall       21
4  07227500 Chloride flow-adjusted seasonal Kendall       21
5  07228000  Calcium    uncensored seasonal Kendall       21
6  07228000  Calcium flow-adjusted seasonal Kendall       21
7  07228000 Chloride    uncensored seasonal Kendall       21
8  07228000 Chloride flow-adjusted seasonal Kendall       21
9  07297910  Calcium    uncensored seasonal Kendall       21
10 07297910  Calcium flow-adjusted seasonal Kendall       21
11 07297910 Chloride    uncensored seasonal Kendall       21
12 07297910 Chloride flow-adjusted seasonal Kendall       21
13 07300000  Calcium    uncensored seasonal Kendall       21
14 07300000  Calcium flow-adjusted seasonal Kendall       21
15 07300000 Chloride    uncensored seasonal Kendall       21
16 07300000 Chloride flow-adjusted seasonal Kendall       21
17 07308500  Calcium    uncensored seasonal Kendall       21
18 07308500  Calcium flow-adjusted seasonal Kendall       21
19 07308500 Chloride    uncensored seasonal Kendall       21
20 07308500 Chloride flow-adjusted seasonal Kendall       21
21 07316000  Calcium    uncensored seasonal Kendall       21
22 07316000  Calcium flow-adjusted seasonal Kendall       21
23 07316000 Chloride    uncensored seasonal Kendall       21
24 07316000 Chloride flow-adjusted seasonal Kendall       21
25 07331600  Calcium    uncensored seasonal Kendall       21
26 07331600  Calcium flow-adjusted seasonal Kendall       21
27 07331600 Chloride    uncensored seasonal Kendall       21
28 07331600 Chloride flow-adjusted seasonal Kendall       21
29 07336820  Calcium    uncensored seasonal Kendall       21
30 07336820  Calcium flow-adjusted seasonal Kendall       21
31 07336820 Chloride    uncensored seasonal Kendall       21
32 07336820 Chloride flow-adjusted seasonal Kendall       21
33 07342500  Calcium    uncensored seasonal Kendall       21
34 07342500  Calcium flow-adjusted seasonal Kendall       21
35 07342500 Chloride    uncensored seasonal Kendall       21
36 07342500 Chloride flow-adjusted seasonal Kendall       21
37 07343000  Calcium    uncensored seasonal Kendall       21
38 07343000  Calcium flow-adjusted seasonal Kendall       21
```

```
39 07343000 Chloride    uncensored seasonal Kendall       21
40 07343000 Chloride flow-adjusted seasonal Kendall       21
41 07343200  Calcium    uncensored seasonal Kendall       21
42 07343200  Calcium flow-adjusted seasonal Kendall       21
43 07343200 Chloride    uncensored seasonal Kendall       21
44 07343200 Chloride flow-adjusted seasonal Kendall       21
45 07343500  Calcium    uncensored seasonal Kendall       21
46 07343500  Calcium flow-adjusted seasonal Kendall       21
47 07343500 Chloride    uncensored seasonal Kendall       21
48 07343500 Chloride flow-adjusted seasonal Kendall       21
49 07344500  Calcium    uncensored seasonal Kendall       21
50 07344500  Calcium flow-adjusted seasonal Kendall       21
51 07344500 Chloride    uncensored seasonal Kendall       21
52 07344500 Chloride flow-adjusted seasonal Kendall       21
53 07346070  Calcium    uncensored seasonal Kendall       21
54 07346070  Calcium flow-adjusted seasonal Kendall       21
55 07346070 Chloride    uncensored seasonal Kendall       21
56 07346070 Chloride flow-adjusted seasonal Kendall       21
   NumSeas Nobs   RepValue       Trend    Trend.pct      P.value
1        6  123  100.00001  0.00000000  0.000000000 0.8336014152
2        6  123  100.00001 -0.03341340 -0.033413399 0.9601243138
3        6  124  469.89363 12.79590098  2.723148421 0.0336792469
4        6  124  469.89363 12.63865246  2.689683714 0.0129020214
5        6  111  110.00001  2.39588639  2.178078333 0.0003365278
6        6  111  110.00001  1.28919788  1.171997963 0.0138536692
7        6  111  660.00008 17.25881435  2.614971565 0.0007134676
8        6  111  660.00008 11.38146508  1.724464204 0.0029419661
9        6  122  530.00011  1.38744659  0.261782321 0.8355770111
10       6  122  530.00011  4.00436597  0.755540591 0.2681846619
11       6  122 3000.00035 30.77328679  1.025776108 0.8205802441
12       6  122 3000.00035 82.04729202  2.734909417 0.0758367777
13       6  123  480.00003  0.00000000  0.000000000 0.8724372387
14       6  123  480.00003 -0.04017926 -0.008370679 0.9429429173
15       6  123  270.00002  2.26912466  0.840416463 0.0046260357
16       6  123  270.00002  2.26199816  0.837777018 0.0180431604
17       6  119  340.00001 -0.87151697 -0.256328516 0.6151251197
18       6  119  340.00001 -1.02378192 -0.301112325 0.5201364756
19       6  119 1837.99988  8.02723876  0.436737719 0.5162076950
20       6  119 1837.99988 -3.46897676 -0.188736506 0.8067187071
21      12  182  200.00001  0.69571531  0.347857631 0.5388302803
22      12  182  200.00001  2.10377018  1.051885022 0.1010135412
23      12  188 1000.00010  9.27514624  0.927514535 0.3566403389
24      12  188 1000.00010 18.19829793  1.819829619 0.0474613905
25      12  200   88.49858  0.62565134  0.706962055 0.2394109964
26      12  200   88.49858  0.38069780  0.430173928 0.3169723749
27      12  203  320.00001  2.57714511  0.805357813 0.5003621578
28      12  203  320.00001  0.68797344  0.214991690 0.7803473473
29      12  185   65.00001  0.84057835  1.293197225 0.0961654186
30      12  185   65.00001  0.66272802  1.019581383 0.1187556982
31      12  188  166.49328  4.10125215  2.463313924 0.0698596239
32      12  188  166.49328  3.75636327  2.256165094 0.0728764534
```

```
33      12  183   40.00000 -0.35416765 -0.885419081 0.2286658287
34      12  183   40.00000 -0.30501864 -0.762546581 0.1911620051
35      12  183   16.00000 -0.31416803 -1.963550197 0.1585604995
36      12  183   16.00000 -0.16485555 -1.030347162 0.2915501893
37      12  170   79.49842  0.20723170  0.260673977 0.6322352886
38      12  170   79.49842 -0.18727827 -0.235574825 0.6346129775
39      12  170   35.00000 -0.16173531 -0.462100829 0.7745313048
40      12  170   35.00000 -0.57496763 -1.642764493 0.0628329962
41      12  184   55.99999 -0.40639101 -0.725698359 0.2162646502
42      12  184   55.99999 -0.56940542 -1.016795562 0.0369244702
43      12  184   21.00000 -0.58466480 -2.784117838 0.0263182856
44      12  184   21.00000 -0.53588794 -2.551847132 0.0054894532
45      12  179   14.00000 -0.07162687 -0.511620472 0.5025991797
46      12  179   14.00000 -0.05776933 -0.412638017 0.3829599321
47      12  179   20.00000 -0.32744925 -1.637246215 0.2295798212
48      12  179   20.00000 -0.32282345 -1.614117195 0.0948637649
49      12  186   16.00000 -0.09071358 -0.566959859 0.2795946300
50      12  186   16.00000 -0.12641082 -0.790067630 0.0304778069
51      12  186   44.49719 -0.49735710 -1.117726880 0.3637532592
52      12  186   44.49719 -0.94315144 -2.119575081 0.0002551555
53      12  183    7.00000 -0.04453901 -0.636271629 0.0876174122
54      12  183    7.00000 -0.05662205 -0.808886448 0.0062053259
55      12  183   30.00000 -0.70519603 -2.350653317 0.0265707411
56      12  183   30.00000 -0.71815740 -2.393857888 0.0005073280
   Trend.dir
1          *
2       none
3         up
4         up
5         up
6         up
7         up
8         up
9       none
10      none
11      none
12      none
13         *
14      none
15        up
16        up
17      none
18      none
19      none
20      none
21      none
22      none
23      none
24        up
25      none
26      none
```

27	none
28	none
29	none
30	none
31	none
32	none
33	none
34	none
35	none
36	none
37	none
38	none
39	none
40	none
41	none
42	down
43	down
44	down
45	none
46	none
47	none
48	none
49	none
50	down
51	none
52	down
53	none
54	down
55	down
56	down

7 Further Remarks

Because trend analysis is not necessarily a straightforward process, but requires user assessments at several points in the process, it is not necessarily a good idea to simply create scripts and run them without any user review and interaction. To overcome recording the steps in a script, the functions in restrend record all changes to the projects database in a list called `estrend.cl`. It can be viewed at any time simply by entering estrend.cl in the console window. It can be saved with the data to ensure that the trend analysis is reproducible.

```
> # get the history
> estrend.cl

[[1]]
setProj(project = "majors", data = Majors, STAID = "STAID", DATES = "DATES",
    Snames = c("Calcium", "Chloride"), FLOW = "FLOW", type = "seasonal",
    Start = "1968-10-01", End = "1989-10-01")

[[2]]
flowAdjust()

[[3]]
flowAdjust(Stations = "07331600", Snames = c("Calcium", "Chloride"),
    span = 1)

[[4]]
SKTrends()
```

References

[1] Lorenz, D.L., in preparation, restrend: an R package for EStimate TRENDs: U.S. Geological Survey Open File Report, ? p.

[2] Schertz, T.L., Alexander, R.B., and Ohe, D.J., 1991, The computer program EStimate TREND (ESTREND), a system for the detection of trends in water-quality data: U.S. Geological Survey Water Resources Investigations Report 91-4040, 72 p.