Nondetects And Data Analysis:
Trend Analysis with NDs

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Practical Stats

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Trend Analysis Methods

	Time only X var	Time + Covariate	Seasonal
Parametric	1 MLE Simple Regression cencorreg (y, ycen, x)	2 MLE Multiple Regression cencorreg (y, ycen, x.frame)	3 MLE Regression with sin and cos terms cencorreg (y, ycen, x.frame)
Nonparametric	4 Akritas-Theil-Sen ATS (y, ycen, time)	5 ATS on residuals from a GAM smooth centrend (y, ycens, x, time)	6 Censored Seasonal-Kendall test censeaken (y, ycen, time, season)

None of these methods substitute a number like DL/2 for nondetects

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R packages required

If you haven't already installed and loaded these three R packages:

cenGAM, mgcv, nlme

you will need to install and load them before you can perform the 3 nonparametric methods in this Section.

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Parametric Trend Analysis

Censored regression solved by Maximum Likelihood Estimation (MLE) -- cencorreg function

1. Check for multicollinearity between X variables
2. Use the cencorreg script to compute the regression equation
3. Check that residuals follow the assumed distribution
4. When comparing models, choose the one with the lowest AIC

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Example Data

DairyCreekCr.Rdata includes Total Recoverable Chromium concentrations (some nondetects) and dectime (decimal time) for the day of sampling. Provided by a colleague.

Note: Data have been altered from the original (I filled in some flow data so fewer were missing).

Censoring indicator variable (here CrND distinguishes 1 = a detection limit in the Y column from 0 = detected concentration in the Y column.

To perform a simple regression (only dectime as the X variable), use the cencorreg script from the regression section:

```
> cencorreg(`Total Recoverable Chromium`, CrND, dectime)
```

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1 Simple Regression
(one X variable -- time)

```
> cencorreg(`Total Recoverable Chromium`, CrND, dectime)
 Likelihood R = -0.339                    AIC = 96.39843
 Rescaled Likelihood R = -0.3824          BIC = 101.8751
 McFaddens R = -0.2815
Call: survreg(formula = "log(Total Recoverable Chromium)", data = "dectime",
    dist = "gaussian")
```

NOTE: default is to use log(Y)

```
Coefficients:
(Intercept)    dectime
119.7497387 -0.0596987
Scale= 0.4767561
Loglik(model)= -44.7   Loglik(intercept only)= -48.5
     Chisq= 7.69 on 1 degrees of freedom, p= 0.00555
n= 63
```

The slope is significant (p = 0.005) showing a decrease of 0.059 log units per year.

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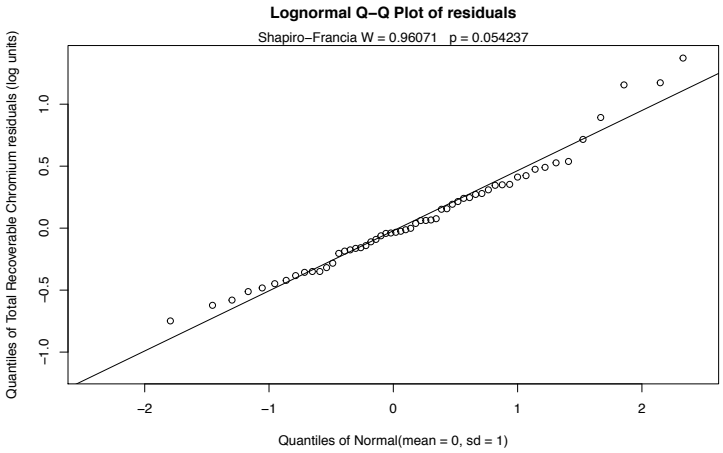
Check Normality of Residuals

Do not reject normality using log(Cr)



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2 Multiple Regression, X and Time

Regression using both flow and dectime as explanatory variables. To do multiple regression using cencorreg, input the x variables as a single data frame. Create the data frame for both variables, then run the model:

```
> xvar2 <- data.frame(dectime, mean_daily_flow_cfs)
> reg.cr <- cencorreg(`Total Recoverable Chromium`, CrND, xvar2)
 Likelihood R2 = 0.4617                    AIC = 63.5293
 Rescaled Likelihood R2 = 0.5846           BIC = 70.83945
 McFaddens R2 = 0.3971
> summary(reg.cr)
```

smaller than the 1-variable model, so this is better

(see next slide)

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2 MLE Regression Results

```
> summary(reg.cr)
Call:
survreg(formula = "log(Total Recoverable Chromium)", data = "dectime+mean_daily_flow_cfs",
    dist = "gaussian")
                       Value Std. Error      z       p
(Intercept)         1.02e+02   3.31e+01   3.09  0.0020.
dectime            -5.11e-02   1.64e-02  -3.11  0.0019
mean_daily_flow_cfs 6.19e-04   9.89e-05   6.26 3.9e-10
Log(scale)         -1.01e+00   1.01e-01 -10.03 < 2e-16
Scale= 0.362

Gaussian distribution
Loglik(model)= -27.3   Loglik(intercept only)= -45.2
    Chisq= 35.92 on 2 degrees of freedom, p= 1.6e-08
n=58 (5 observations deleted due to missingness)
```

Downtrend of 0.051 log units per year. Adj for flow

Significant increase in log(Cr) with flow

Overall significant model

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Always check that VIFs < 10

```
> vif(lm(`Total Recoverable Chromium`~ dectime + mean_daily_flow_cfs))
          dectime mean_daily_flow_cfs
         1.000662            1.000662
```

No multicollinearity present

You may use the lm command for uncensored regression because vifs do not have anything to do with the Y variable. They just measure the multicollinearity (multiple correlations) between the X variables.

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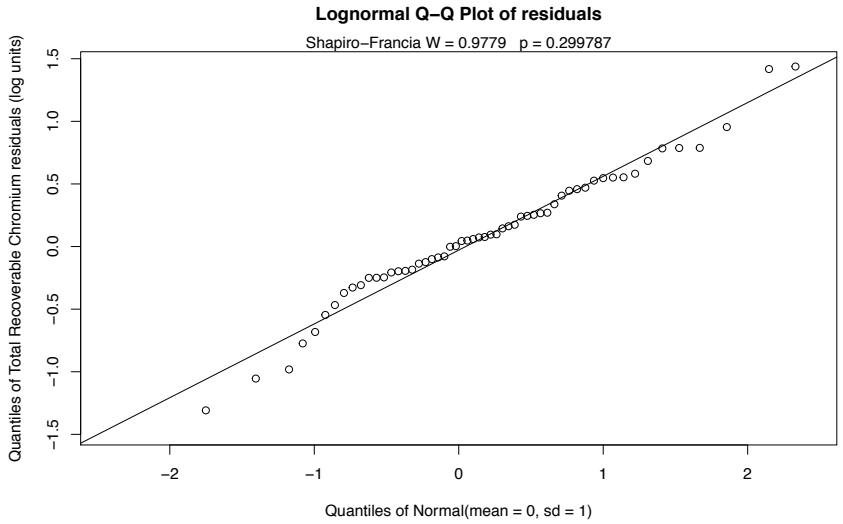
Always Check Normality of Residuals

Do not reject normality of residuals from the multiple regression using log(Cr)



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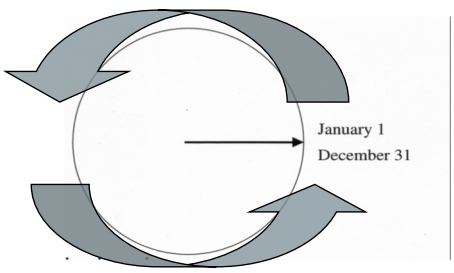
3 Seasonal Regression with sine and cosine

Two new explanatory variables are created, and added to the regression equation

These are the sine and cosine of $2\pi T$, where T is time in decimal years (1997.5)

Resulting in one revolution every year … $2\pi T$



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3 Regression with sine and cosine

$$Y = b_0 + b_1*T + b_2*X + b_3*\sin(2\pi T) + b_4*\cos(2\pi T)$$

- Keep both sin and cos seasonal terms, or keep neither.
- Base the decision on significance of b_3, b_4.
- If either are significantly different than zero, keep both terms.
- You can instead compare the AIC for models with and without the sin and cos terms. The model with the lowest AIC is better.

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3 Regression with sine and cosine

```
> cosT <- cos(2*pi*dectime)
> sinT <- sin(2*pi*dectime)
> xvar4 <- data.frame(dectime, mean_daily_flow_cfs, sinT, cosT)

> reg4 <- cencorreg(`Total Recoverable Chromium`, CrND, xvar4)
 Likelihood R2 = 0.4645                    AIC = 67.22336
 Rescaled Likelihood R2 = 0.5882           BIC = 78.68859
 McFaddens R2 = 0.4005
```

AIC was 63.53 without sine and cosine, so the 2 variable model was better.

No significant seasonal variation

continued on next slide:

```
> vif(lm(`Total Recoverable Chromium`~ dectime + mean_daily_flow_cfs + sinT + cosT))
            dectime     mean_daily_flow_cfs                    sint                    cost
           1.008583                2.555278             1.883205             1.596627
```

No multicollinearity problems

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3 Regression with sine and cosine

```
survreg(formula = "log(Total Recoverable Chromium)", data = "dectime+mean_daily_flow_cfs+sinT+cosT",
    dist = "gaussian")

                      Value Std. Error      z       p
(Intercept)        1.00e+02   3.31e+01   3.03 0.00241
dectime           -5.02e-02   1.64e-02  -3.05 0.00226
mean_daily_flow_cfs  5.73e-04   1.57e-04   3.64 0.00027
sinT                4.73e-02   8.98e-02   0.53 0.59848
cosT                2.59e-03   8.98e-02   0.03 0.97700
Log(scale)         -1.02e+00   1.01e-01 -10.06 < 2e-16
Scale= 0.361

Gaussian distribution
Loglik(model)= -27.1   Loglik(intercept only)= -45.2
Chisq= 36.23 on 4 degrees of freedom, p= 2.6e-07
n=58 (5 observations deleted due to missingness)
```

Significant down trend in log(Cr)

Significant relation to flow

Not Significant

Not Significant

Conclusion: No seasonal variation.
Use the 2 variable model.

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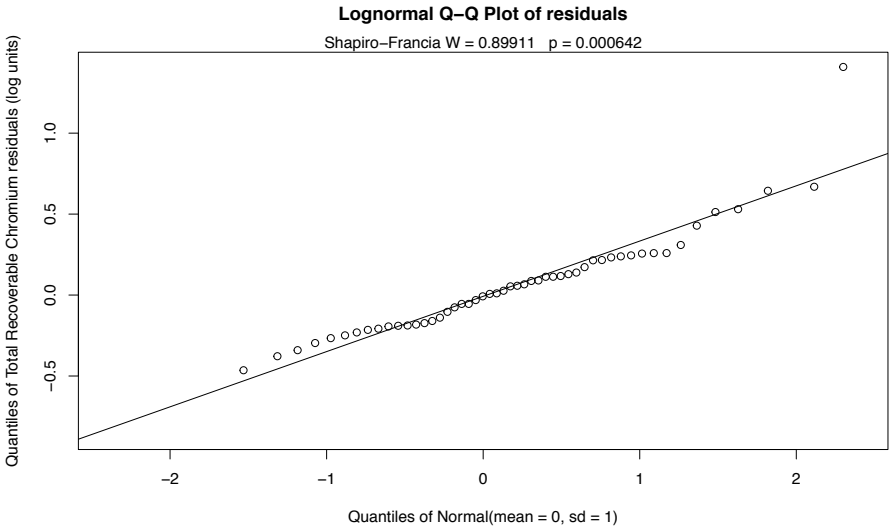
Always Check Normality of Residuals

Reject normality of residuals from the multiple regression. But there's not much else you can do -- its caused by the one large outlier.

Check the value for that outlier but use these units because of the straight line for all but one point.



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Nonparametric Trend Tests with Censored Data

Based on ATS: The Akritas-Theil-Sen line

- Slope is the one that produces a Kendall's tau of 0 for the residuals from the line.
- Test for slope = 0 is the test for Kendall's tau of data vs. time – the Trend Test
- This should sound familiar. See the ATS portion of the regression section.

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4. Simple Nonparametric Regression

```
> ATS(`Total Recoverable Chromium`, CrND, dectime, LOG = FALSE)
Akritas-Theil-Sen line for censored data

Total Recoverable Chromium = 74.2315 -0.0366 * dectime
Kendall's tau = -0.2232   p-value = 0.00979
```

(tau = -0.22 is something like -0.4 for Pearson's r correlation)

There is a significant downtrend. The model is linear over time. So there is a median decrease of 0.0366 ug/L of Chromium per year.

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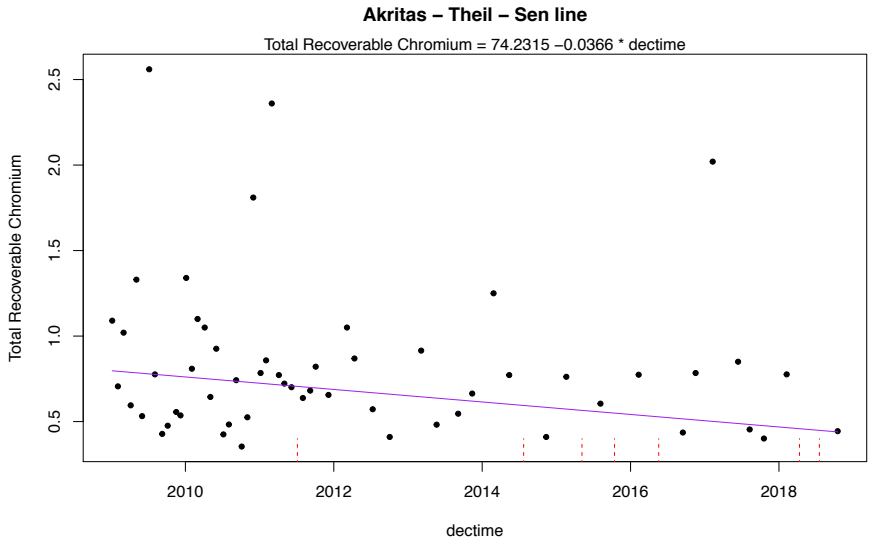
4. ATS line

This test is not strongly affected by outliers. Logs of Cr could be taken instead, producing a curved relationship. Your call. Same p-value.



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5. Nonparametric Trend with a Covariate "multiple regression"

1. Compute a smooth of censored Y vs X, where X is not time, using Generalized Additive Models (GAM)
2. Compute an ATS on the residuals -- Kendall's tau test of change in residuals over time. Slope is still in Y units per time.

- R function centrend (Y, Y.cen, X, time)
- time is often as decimal time (i.e. 2013.5 for halfway through the year)

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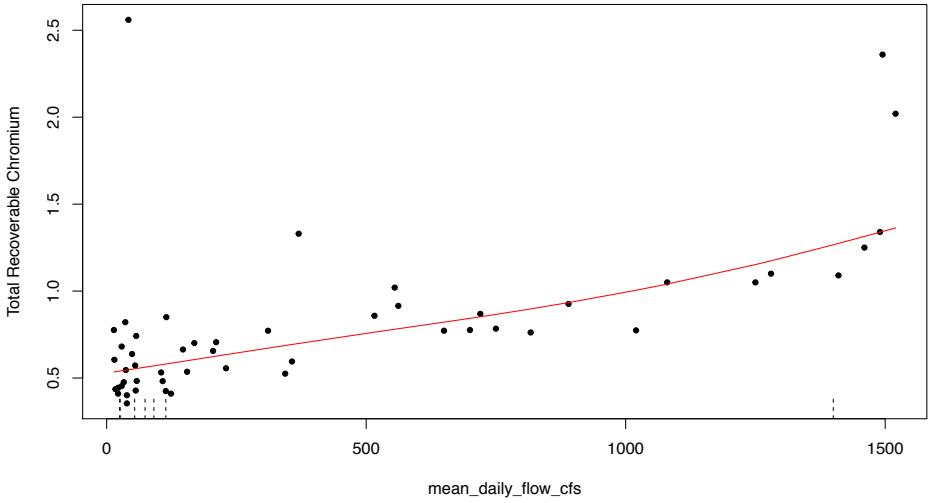
centrend function

```
> resid.trend <- centrend(`Total Recoverable Chromium`, CrND, mean_daily_flow_cfs, dectime)
```

Smooth of Cr concentrations vs. mean daily flow by censored GAM

dashed lines are the censored data



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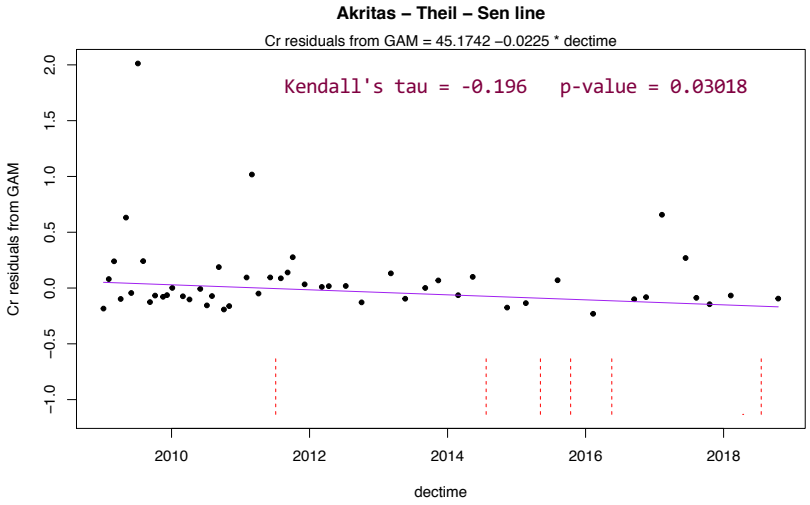
ATS (Mann-Kendall) test on censored GAM residuals

Low censored data (dashed lines) contribute to the test results. Note that they appear mostly at later times, increasing evidence for a downtrend.



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What's a GAM?

Generalized Additive Models

- relate Y to Xs using smooth curves instead of just a linear model
- smooths are a weighted combination of multiple functions
- a smoothing parameter determines how the functions are combined, so that the smoothness can be customized to the need
- Cubic regression splines (the default in centrend) use a cubic regression form (x, x^2, x^3 terms). Multiple cubic regressions are run and combined to maximize smoothness, but not so smooth that a straight line results.

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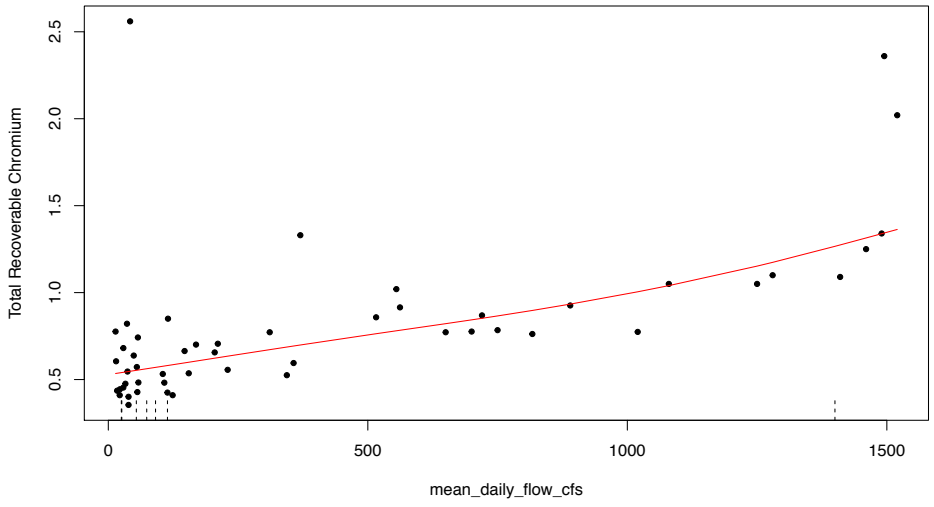
Note that the relationship is not linear

```
> resid.trend <- centrend(`Total Recoverable Chromium`, CrND, mean_daily_flow_cfs, dectime)
```

Smooth of Cr concentrations vs. mean daily flow using a cubic regression spine function



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6. Seasonal Kendall test on censored data

- Computes an ATS line and test for each season separately
- Combines them to produce an overall SK test
- Is a test of 'consistent trend' -- if one season shows a significant increasing trend and a 2nd a significant decreasing trend, these can cancel each other out so that there is no overall significant Seasonal Kendall trend

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Seasonal Kendall test

- Compare all data within the same season to one another
- DO NOT compare data across different seasons
- Akritas-Theil-Sen slope is the slope that produces a zero Kendall's tau correlation coeff. after the line has been subtracted from the data (residuals).

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Computing the Seasonal Kendall test

The test statistic S_i for each season is the "Mann-Kendall test" -- the number of pluses P_i (increases in Y as time increases) minus the number of minuses M_i (decreases in Y as time increases), comparing data only within that season. For season i we have:

$$S_i = P_i - M_i$$

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Seasonal Kendall test statistic S

For the i = 1 to m seasons,

$$S = \sum_{i=1}^{m} S_i$$

S becomes significant as it becomes more and more nonzero

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6. censeaken function

```
> censeaken (dectime, `Total Recoverable Chromium`, CrND, group = Season)

 DATA ANALYZED: Total Recoverable Chromium vs dectime by Season
----------
  Season  N    S    tau      pval intercept    slope
1    Dry 34 -176 -0.314 0.0091337    79.103 -0.03901
----------
  Season  N   S     tau    pval intercept    slope
1    Wet 29 -24 -0.0591 0.66604    24.355 -0.01169
----------
Seasonal Kendall test and Theil-Sen line
   N    S    Tau Pvalue_SK Nreps Intercept    Slope
1 63 -200 -0.207     0.014   999    74.232 -0.03655
----------
```

Significant downtrend in Dry season

No significant trend in Wet season

Significant trend overall. SK slope is -3.6 ug/L per year

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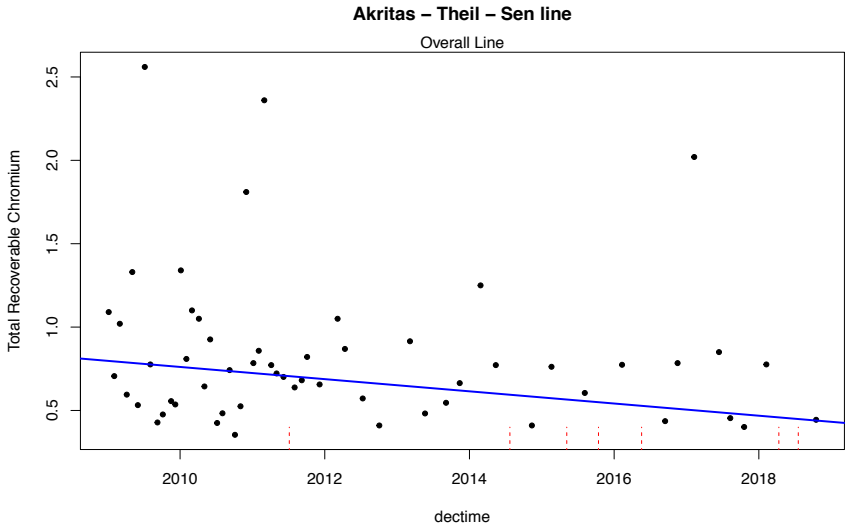
6. censeaken function

Nondetects influence the line and test.

They occur more frequently at later times, adding to the evidence of a downtrend.



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Permutation p-value for the SK test

The SK test without censored data uses a normal approximation to the SK test statistic.
(not a normal assumption for the data, just a smart move by a statistician to form the test statistic)

However the variance of S is not easily computed in a formula when there are censored data. Solution? A permutation test

$$Z_S = \begin{cases} \frac{S-1}{\sqrt{VAR(S)}} & \text{if } S > 0 \\ 0 & \text{if } S = 0 \\ \frac{S+1}{\sqrt{VAR(S)}} & \text{if } S < 0 \end{cases}$$

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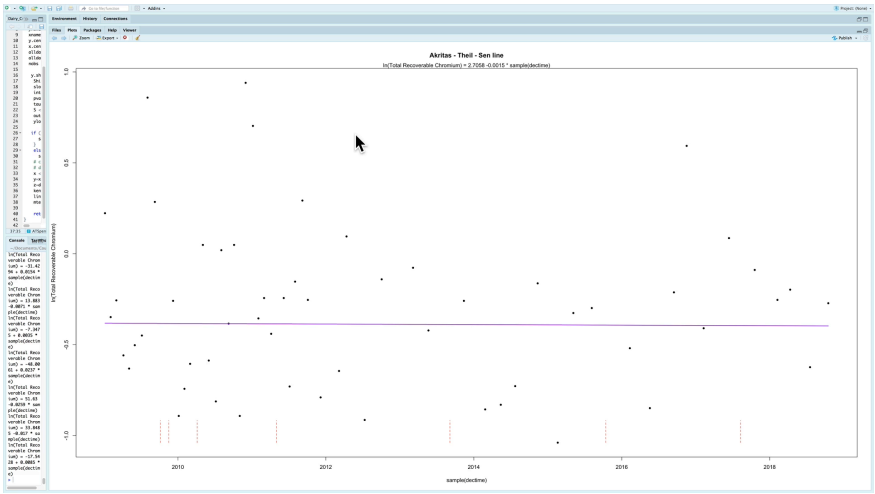
Permutations by shuffling time

The time variable is randomly shuffled 1000s of times and re-assigned to the Y data.

(notice how the times of the nondetect lines change between shuffles)



Then S is computed for each shuffle.

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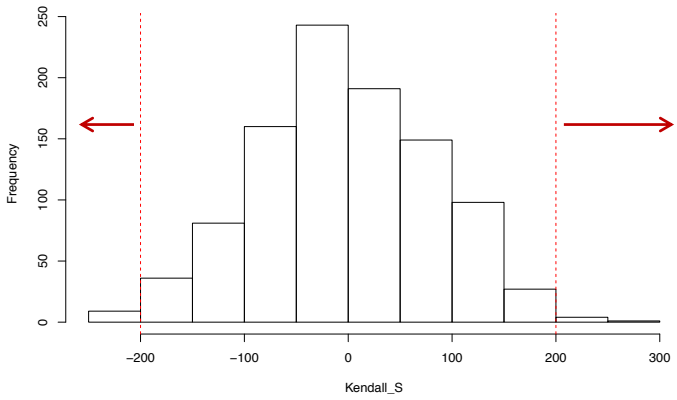
Permutation p-value for the SK test

For each shuffle, the S = P - M test statistic is computed for each season and summed to produce the overall SK S statistic. The collection of the 1000s of SK S statistics put together in one histogram is a picture of the null hypothesis. The p-value is the proportion of times that just by chance the same or greater strength of trend (same S observed from your data) occurs.

For the Dairy Creek data, S = -200.
The proportion that |S| ≥ 200 is the p-value. Here it was 14/1000, or `0.014`

(it may be slightly different the next time)



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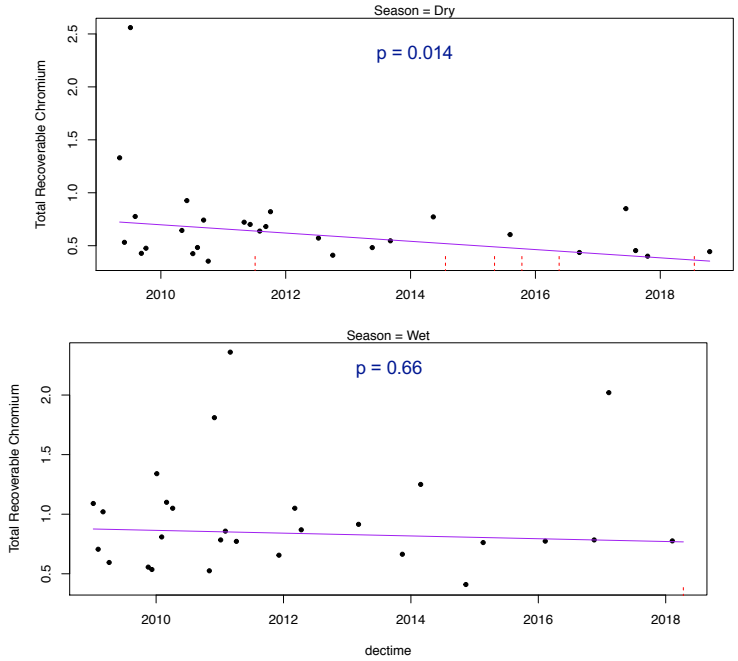
Optional graphs for each season

```
censeaken (dectime, `Total
   Recoverable Chromium`,
   CrND, group = Season,
   seaplots = TRUE)
```



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