

Overview of BayTrends, a CBP software package for Water Quality Trend Detection.

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Talk outline

1. Overview of BayTrends
2. Handling of censored data
3. Modeling of Laboratory methods changes

Key Features of BayTrends:

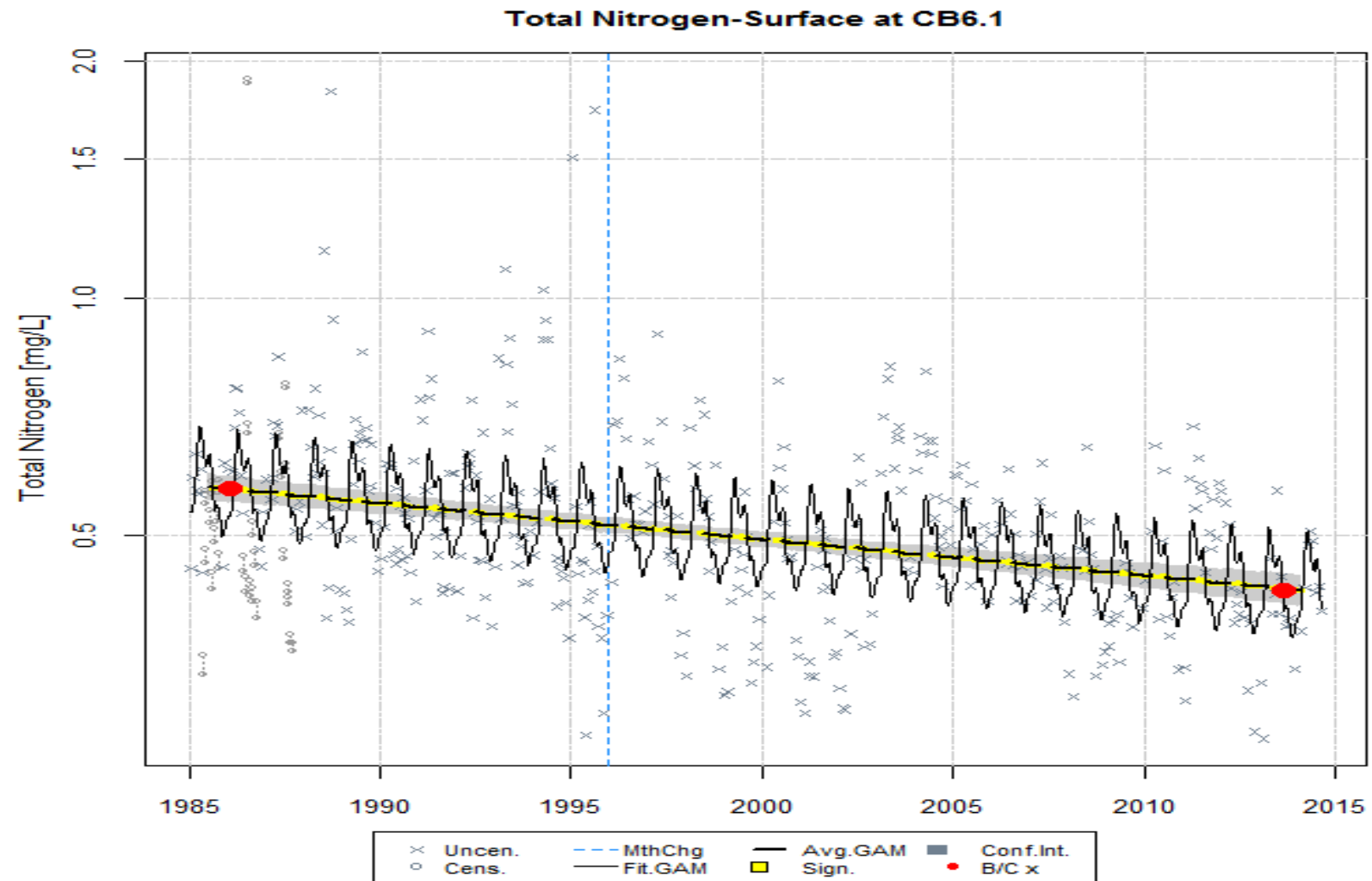
- Written in R, an open source statistical programming environment

- Makes extensive use of Generalized Additive Models (gams)

- Estimates non-monotonic trends

- Does Flow adjustment

Total Nitrogen -- Surface
CB6.1 - S - tn



gam number = 0
 title = Linear Trend with Seasonality
 model = ~ cyear + s(doy,bs='cc')

Table: GAM Analysis of Variance - CB6.1 - S - tn

| type | source | df | F | p.value |
|------------------|---------------|-----------|----------|----------------|
| parametric terms | cyear | 1 | 64.944 | <0.0001 |
| smoothed terms | s(doy) | 7.07 | 9.1123 | <0.0001 |

Table: GAM Parameter Coefficients. - CB6.1 - S - tn

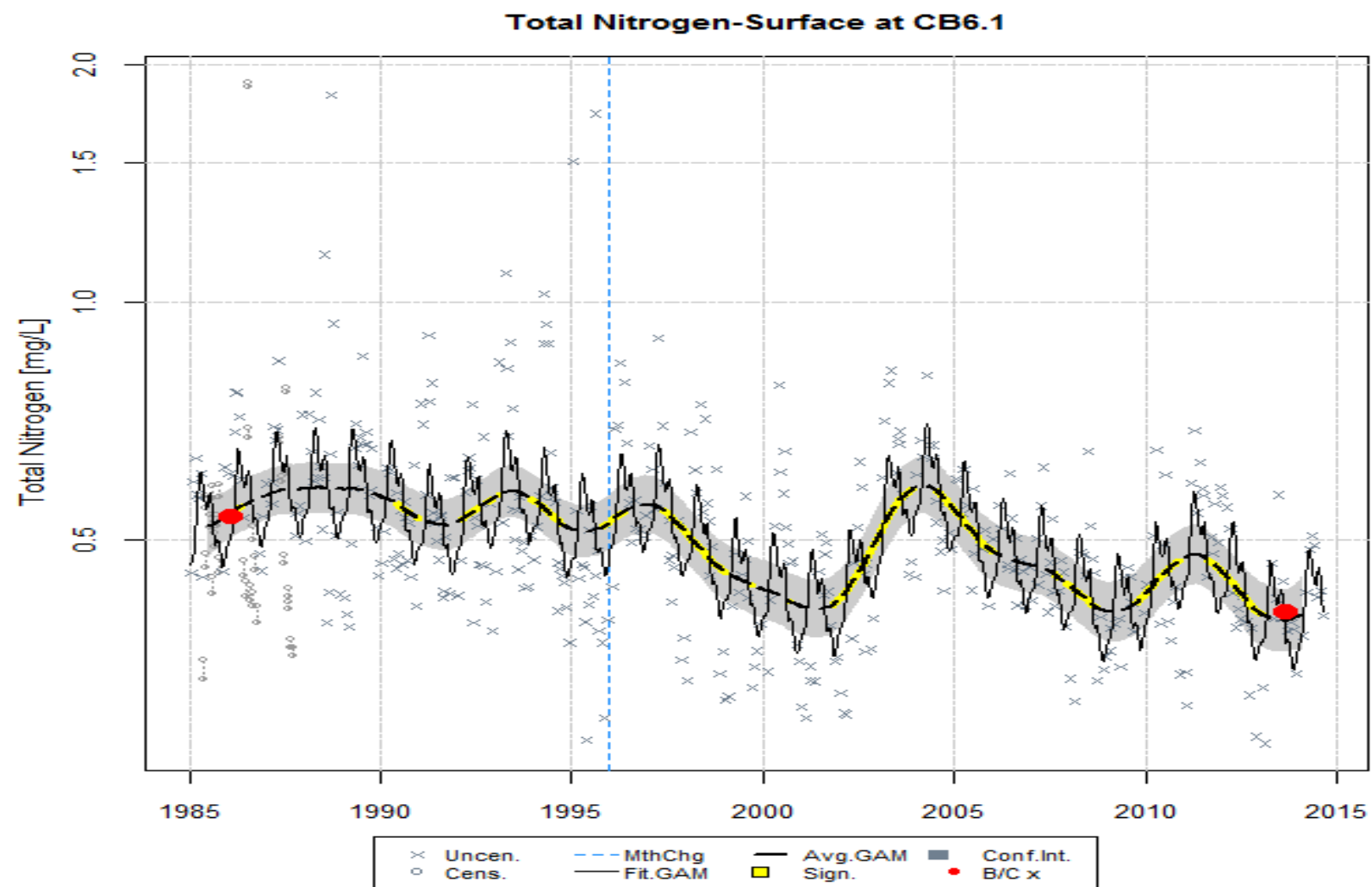
| source | estimate | std.error | t.value | p.value |
|---------------|-----------------|------------------|----------------|----------------|
| (Intercept) | -0.696489 | 0.011518 | -60.4708 | <0.0001 |
| cyear | -0.010527 | 0.001306 | -8.0588 | <0.0001 |

Table: GAM Diagnostics. - CB6.1 - S - tn

| AIC | RMSE | AdjRsquare |
|------------|-------------|-------------------|
| -7.53 | 0.237 | 0.235 |

Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate |
|--|---------------------|
| Baseline log mean (geometric mean) | -0.5571 (0.5729) |
| Current log mean (geometric mean) | -0.8518 (0.4266) |
| Estimated log difference | -0.2948 |
| Std. Err. log difference | 0.0366 |
| 95% Confidence interval for log difference | (-0.3665 , -0.2231) |
| Difference p-value | <0.0001 |
| Period of Record Percent Change Estimate (%) | -25.53% |
| Period of Record | 1985 - 2014 |



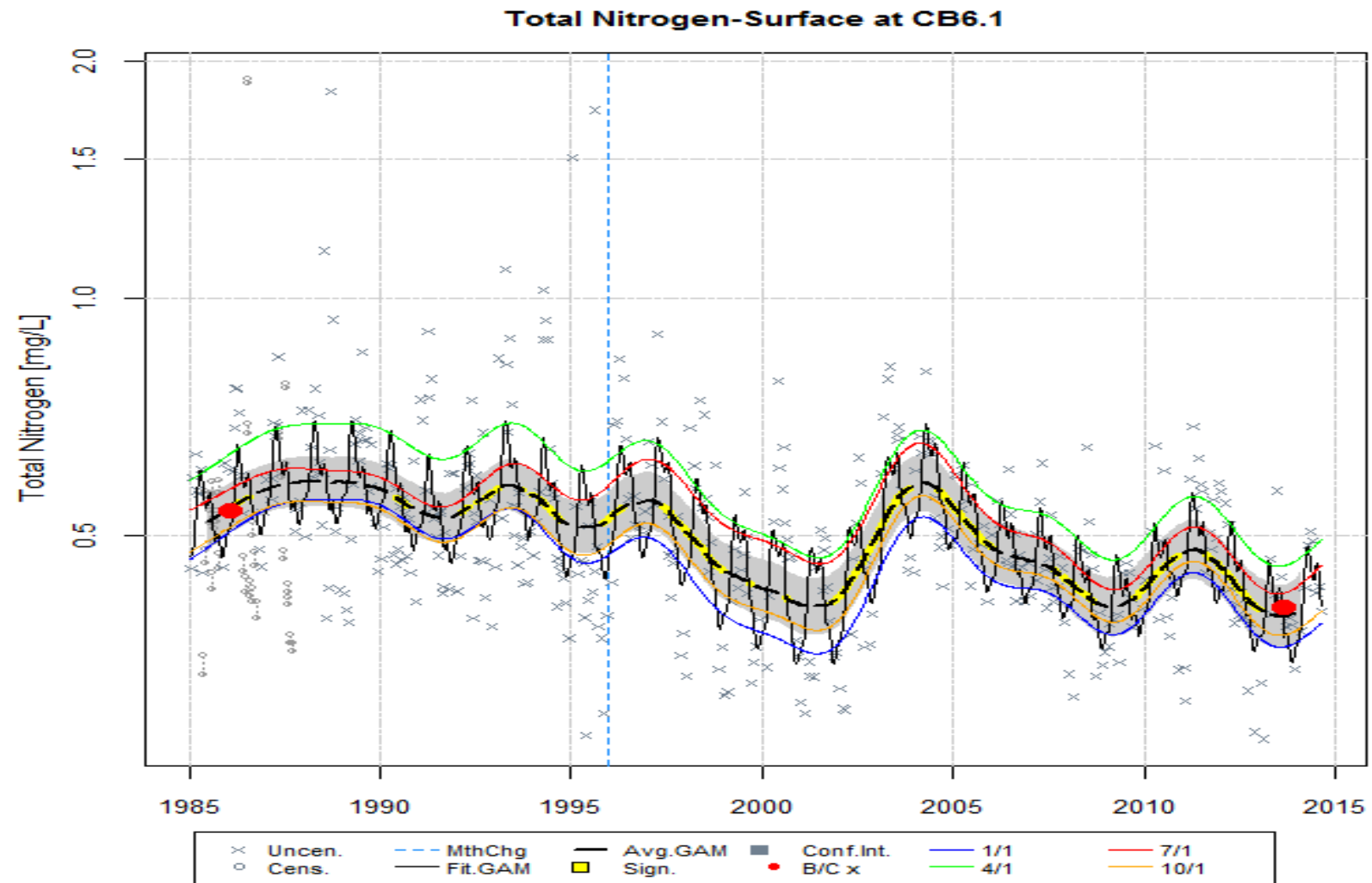
gam number = 1

title = Non-linear Trend with Seasonality

model = \sim cyear + s(cyear, k=gamK1) + s(doy, bs='cc')

Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate |
|--|---------------------|
| Baseline log mean (geometric mean) | -0.623 (0.5363) |
| Current log mean (geometric mean) | -0.9008 (0.4062) |
| Estimated log difference | -0.2778 |
| Std. Err. log difference | 0.0611 |
| 95% Confidence interval for log difference | (-0.3976 , -0.1581) |
| Difference p-value | <0.0001 |
| Period of Record Percent Change Estimate (%) | -24.26% |
| Period of Record | 1985 - 2014 |



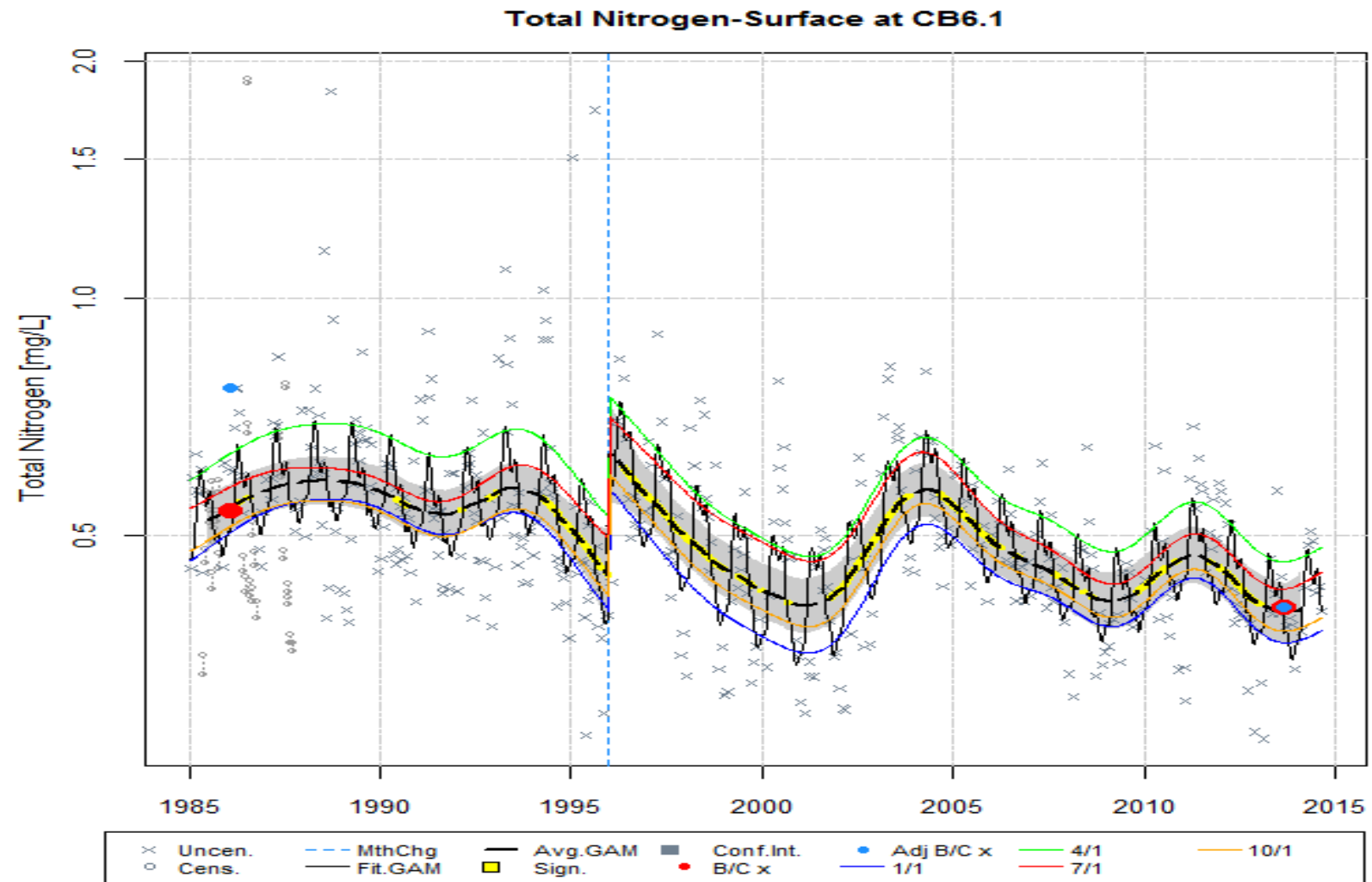
gam number = 2

title = Non-linear trend with Seas+Int

model = ~ cyear + s(cyear, k=gamK1) + s(doy,bs='cc')+ ti(cyear,doy,bs=c('tp','cc'))

Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate |
|--|---------------------|
| Baseline log mean (geometric mean) | -0.6205 (0.5377) |
| Current log mean (geometric mean) | -0.9017 (0.4059) |
| Estimated log difference | -0.2811 |
| Std. Err. log difference | 0.0609 |
| 95% Confidence interval for log difference | (-0.4004 , -0.1619) |
| Difference p-value | <0.0001 |
| Period of Record Percent Change Estimate (%) | -24.51% |
| Period of Record | 1985 - 2014 |



gam number = 3

title = Non-linear trend with Seas+Int. & Intervention

model = ~ intervention + cyear + s(cyear, k=gamK1) + s(doy,bs='cc') + ti(cyear,doy,bs=c('tp','cc'))

Table: GAM Analysis of Variance - CB6.1 - S - tn

| type | source | df | F | p.value |
|------------------|---------------|-----------|----------|----------------|
| parametric terms | intervention | 1 | 8.3066 | 0.0042 |
| " " | cyear | 1 | 2.2368 | 0.1355 |
| smoothed terms | s(cyear) | 14.05 | 4.2546 | <0.0001 |
| " " | s(doy) | 7.02 | 10.1609 | <0.0001 |
| " " | ti(cyear,doy) | 2.55 | 0.5738 | 0.0180 |

Table: GAM Parameter Coefficients. - CB6.1 - S - tn

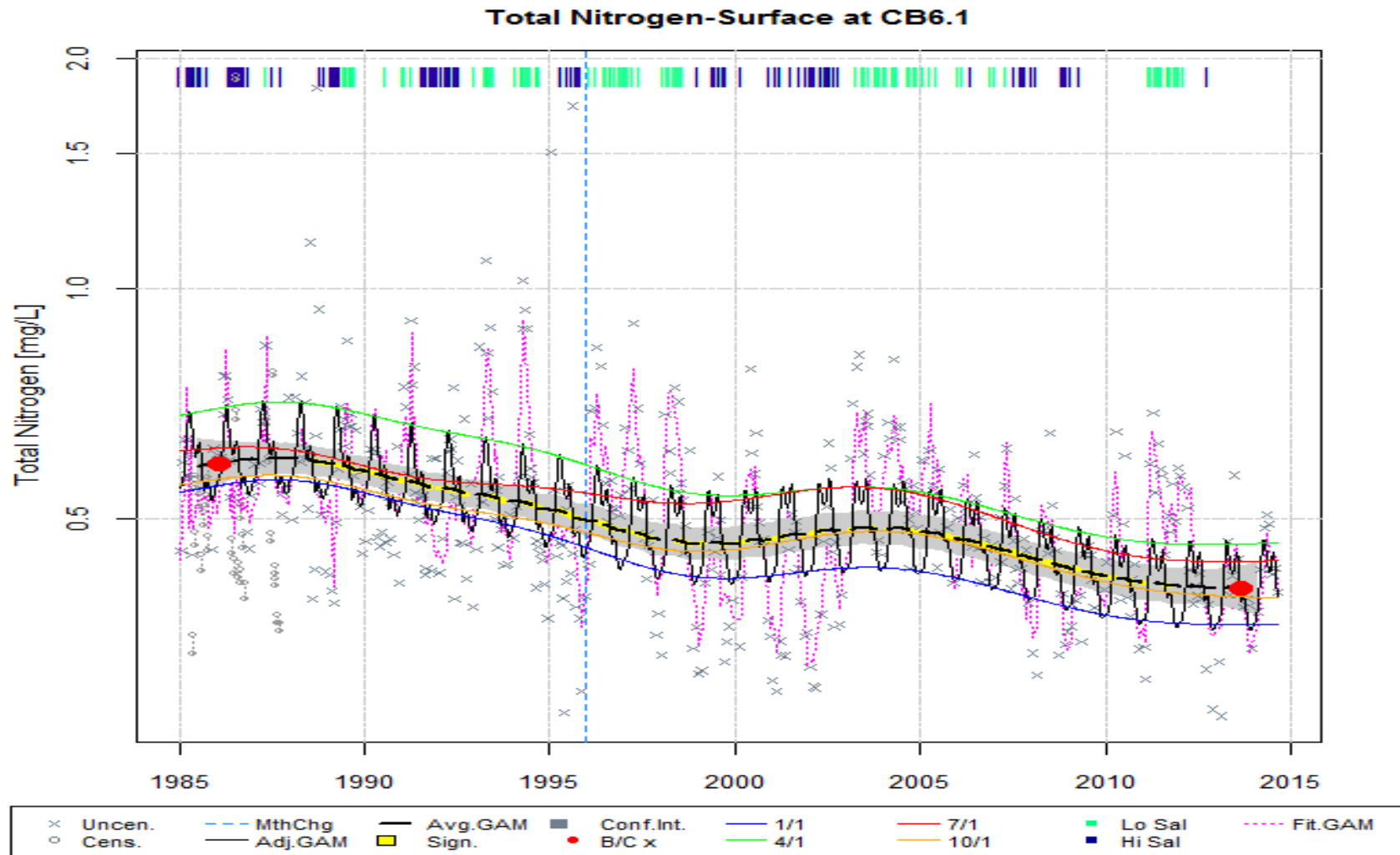
| source | estimate | std.error | t.value | p.value |
|---------------|-----------------|------------------|----------------|----------------|
| (Intercept) | -0.70092 | 0.128784 | -5.4426 | <0.0001 |
| cyear | 0.083596 | 0.055895 | 1.4956 | 0.1355 |
| interventionB | 0.35917 | 0.12462 | 2.8821 | 0.0042 |

Table: GAM Diagnostics. - CB6.1 - S - tn

| AIC | RMSE | AdjRsquare |
|------------|-------------|-------------------|
| -60.22 | 0.2193 | 0.3451 |

Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate | Estimate.Adj |
|--|---------------------|---------------------|
| Baseline log mean (geometric mean) | -0.6202 (0.5378) | -0.2611 (0.7702) |
| Current log mean (geometric mean) | -0.9026 (0.4055) | -0.9026 (0.4055) |
| Estimated log difference | -0.2823 | -0.6415 |
| Std. Err. log difference | 0.0602 | 0.1386 |
| 95% Confidence interval for log difference | (-0.4003 , -0.1644) | (-0.9131 , -0.3699) |
| Difference p-value | <0.0001 | <0.0001 |
| Period of Record Percent Change Estimate (%) | -24.6% | -47.35% |
| Period of Record | 1985 - 2014 | 1985 - 2014 |



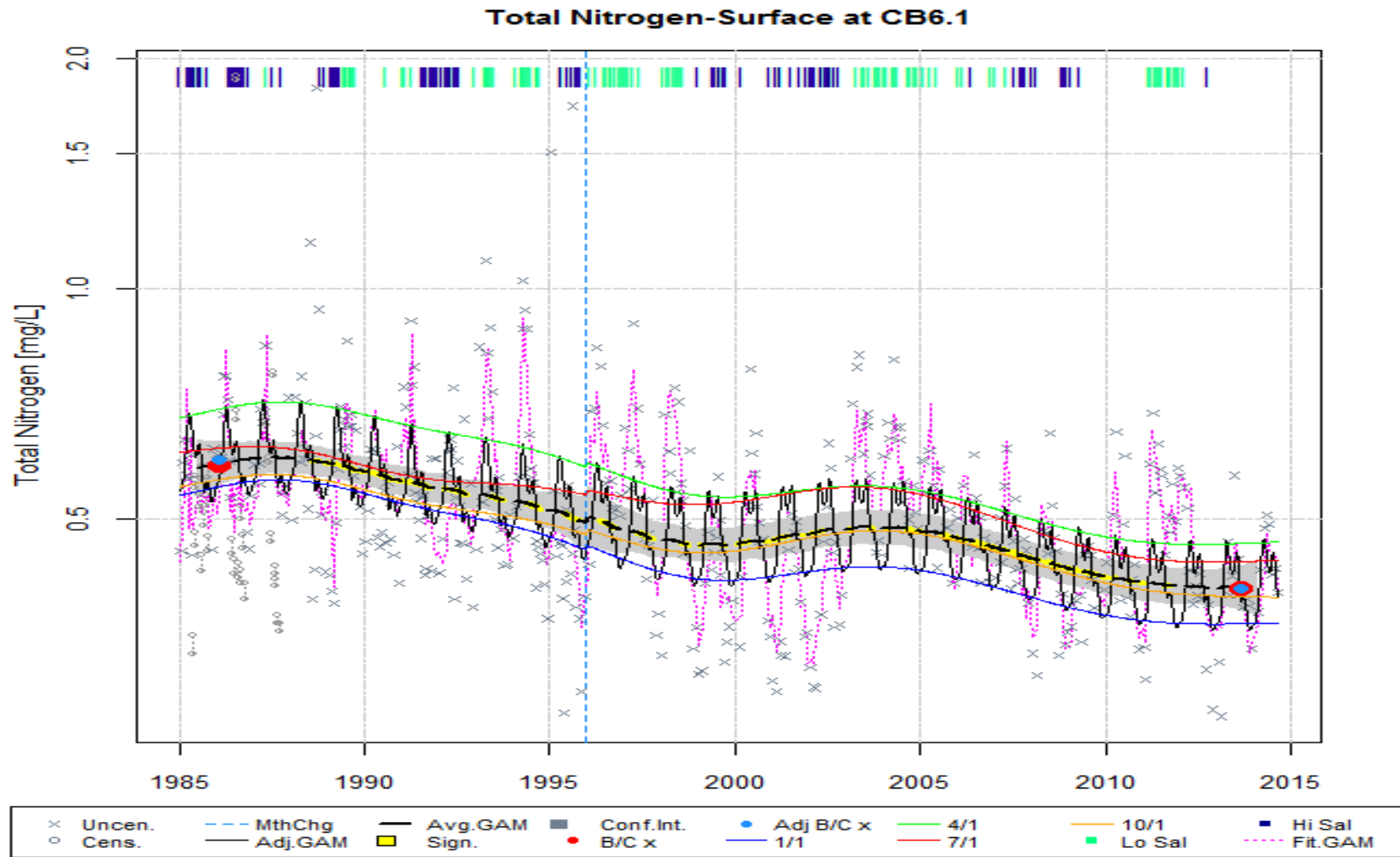
gam number = 4

title = Non-linear trend with Seas+Int. & Hydro Adj

model = ~ cyear + s(cyear, k=gamK1) + s(doy,bs='cc') + ti(cyear,doy,bs=c('tp','cc')) + s(flw_sal,k=gamK2) +
 ti(flw_sal,doy,bs=c('tp','cc')) + ti(flw_sal, cyear,bs=c('tp','tp')) + ti(flw_sal,doy,cyear, bs=c('tp','cc','tp'))

Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate | Estimate.Adj |
|--|---------------------|---------------------|
| Baseline log mean (geometric mean) | -0.5277 (0.5899) | -0.5277 (0.5899) |
| Current log mean (geometric mean) | -0.9021 (0.4057) | -0.9021 (0.4057) |
| Estimated log difference | -0.3744 | -0.3744 |
| Std. Err. log difference | 0.0529 | 0.0529 |
| 95% Confidence interval for log difference | (-0.4782 , -0.2706) | (-0.4782 , -0.2706) |
| Difference p-value | <0.0001 | <0.0001 |
| Period of Record Percent Change Estimate (%) | -31.23% | -31.23% |
| Period of Record | 1985 - 2014 | 1985 - 2014 |



gam number = 5

title = Non-linear trend with Seas+Int., Hydro Adj, & intervention

model = ~ intervention + cyear + s(cyear, k=gamK1) + s(doy, bs='cc') + ti(cyear, doy, bs=c('tp', 'cc')) + s(flw_sal, k=gamK2) + ti(flw_sal, doy, bs=c('tp', 'cc')) + ti(flw_sal, cyear, bs=c('tp', 'tp')) + ti(flw_sal, doy, cyear, bs=c('tp', 'cc', 'tp'))

Table: GAM Analysis of Variance - CB6.1 - S - tn

| type | source | df | F | p.value | Note |
|------------------|-----------------------|-----------|----------|----------------|-------------|
| parametric terms | intervention | 1 | 0.0358 | 0.8500 | - |
| " " | cyear | 1 | 2.8711 | 0.0909 | - |
| smoothed terms | s(cyear) | 5.8 | 2.6853 | 0.0109 | - |
| " " | s(doy) | 7.21 | 12.5699 | <0.0001 | - |
| " " | ti(cyear,doy) | 3.64 | 0.9638 | 0.0017 | - |
| " " | s(flw_sal) | 1 | 134.027 | <0.0001 | - |
| " " | ti(flw_sal,doy) | 4.71 | 3.063 | <0.0001 | - |
| " " | ti(flw_sal,cyear) | 4.09 | 1.0167 | 0.4201 | - |
| " " | ti(flw_sal,doy,cyear) | 0 | 0.0001 | 0.2340 | - |

Table: GAM Parameter Coefficients. - CB6.1 - S - tn

| source | estimate | std.error | t.value | p.value |
|---------------|-----------------|------------------|----------------|----------------|
| (Intercept) | -0.629795 | 0.050984 | -12.3527 | <0.0001 |
| cyear | 0.02825 | 0.016672 | 1.6944 | 0.0909 |
| interventionB | 0.014572 | 0.077027 | 0.1892 | 0.8500 |

Table: GAM Diagnostics. - CB6.1 - S - tn

| AIC | RMSE | AdjRsquare |
|------------|-------------|-------------------|
| -202.2 | 0.1864 | 0.5275 |

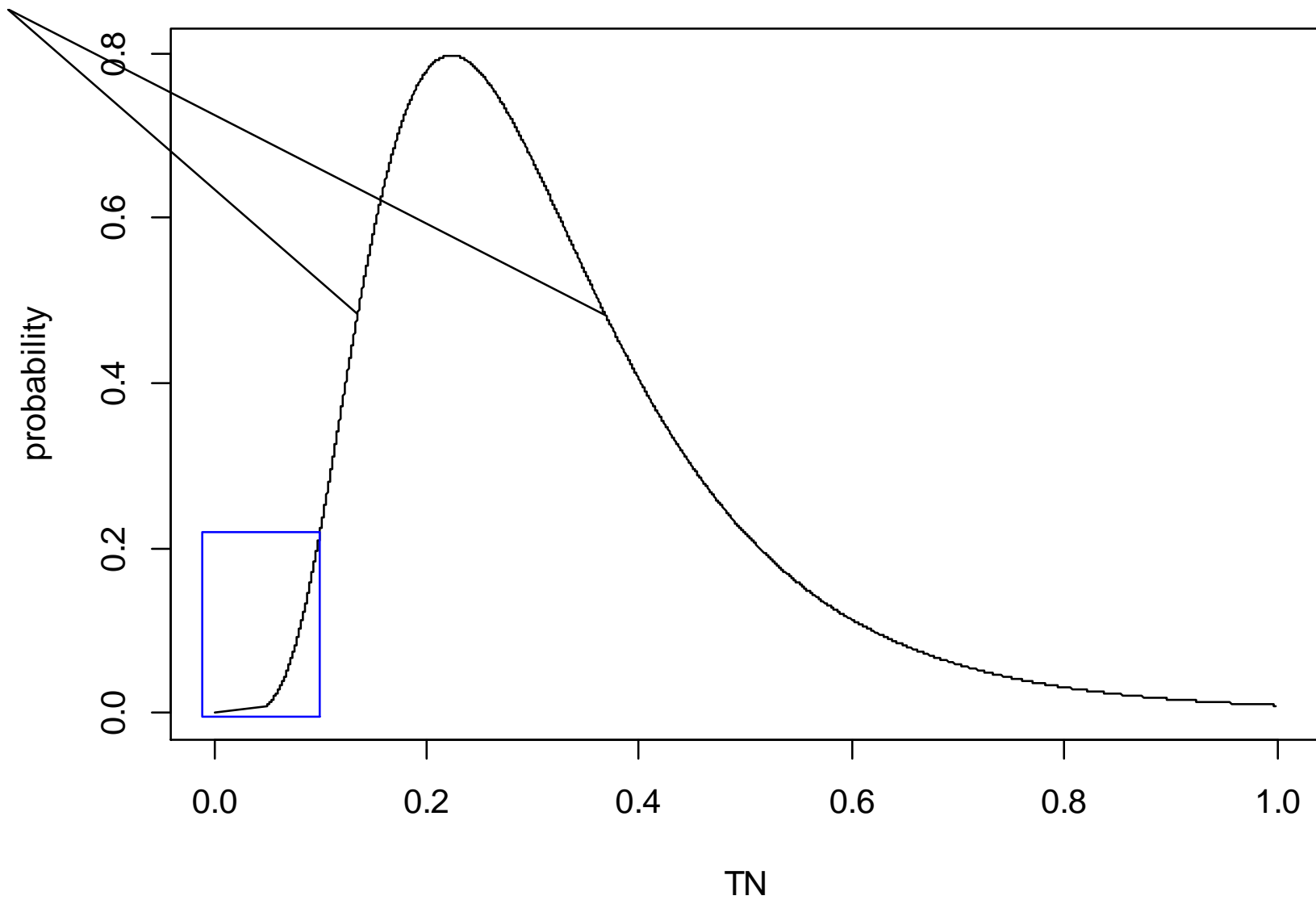
Table: Estimates of Change from 1986-2016. - CB6.1 - S - tn

| Calculation | Estimate | Estimate.Adj |
|--|---------------------|---------------------|
| Baseline log mean (geometric mean) | -0.5299 (0.5887) | -0.5154 (0.5973) |
| Current log mean (geometric mean) | -0.9004 (0.4064) | -0.9004 (0.4064) |
| Estimated log difference | -0.3705 | -0.385 |
| Std. Err. log difference | 0.0534 | 0.0942 |
| 95% Confidence interval for log difference | (-0.4751 , -0.2658) | (-0.5696 , -0.2005) |
| Difference p-value | <0.0001 | <0.0001 |
| Period of Record Percent Change Estimate (%) | -30.96% | -31.96% |
| Period of Record | 1985 - 2014 | 1985 - 2014 |

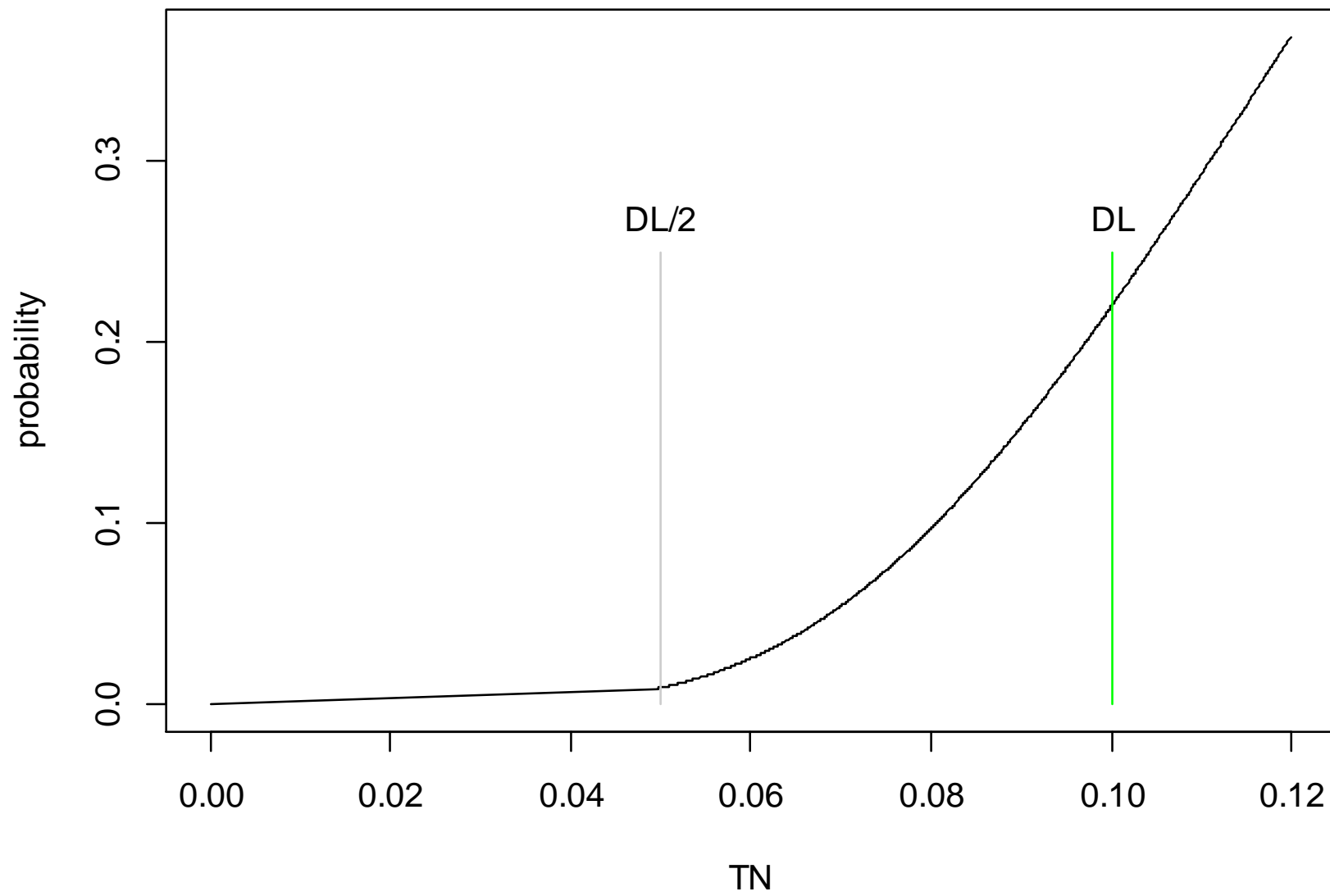
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Censored Data Handling

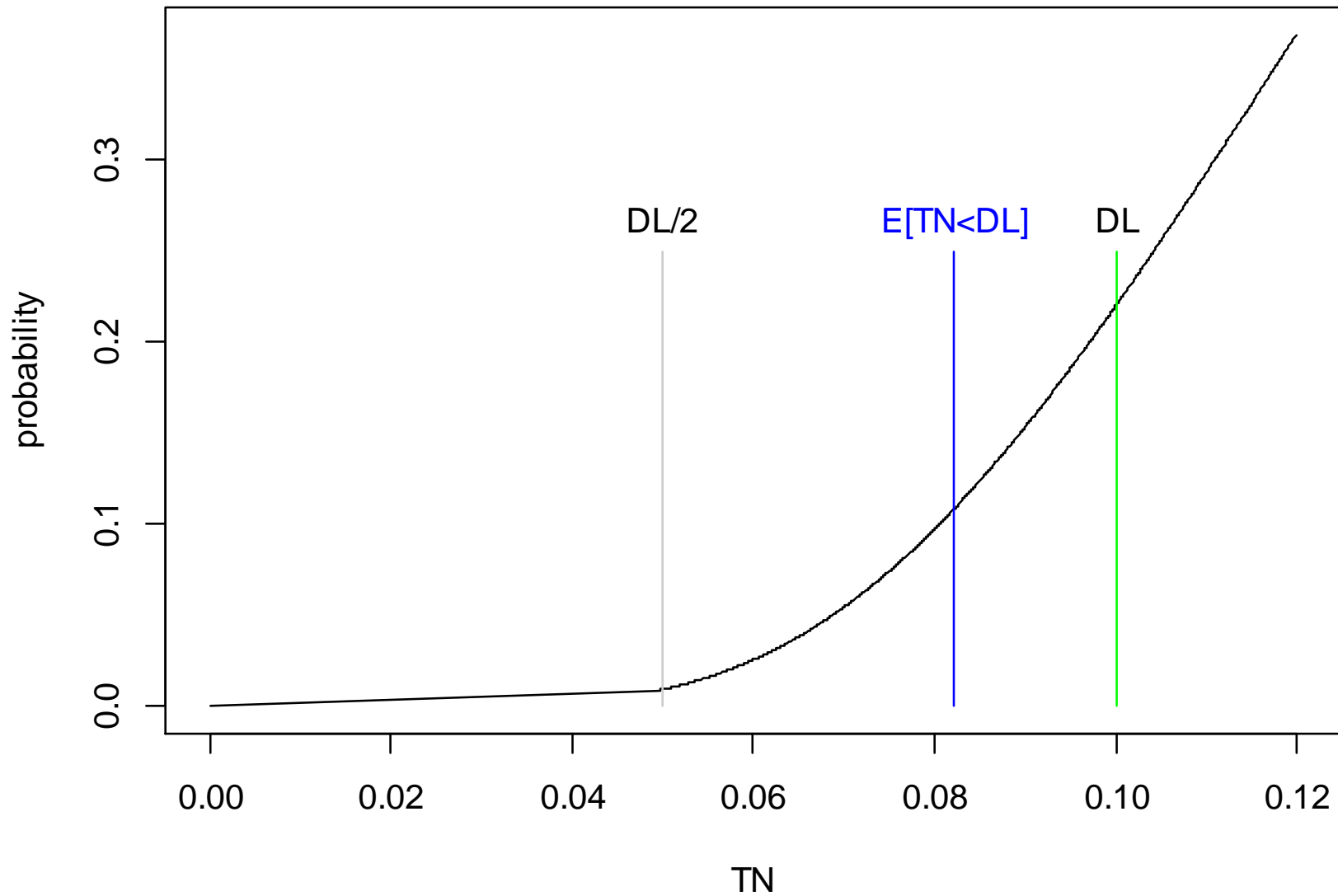
Expectation Maximization Algorithm (EM algorithm)



Assume a log-normal Distribution.

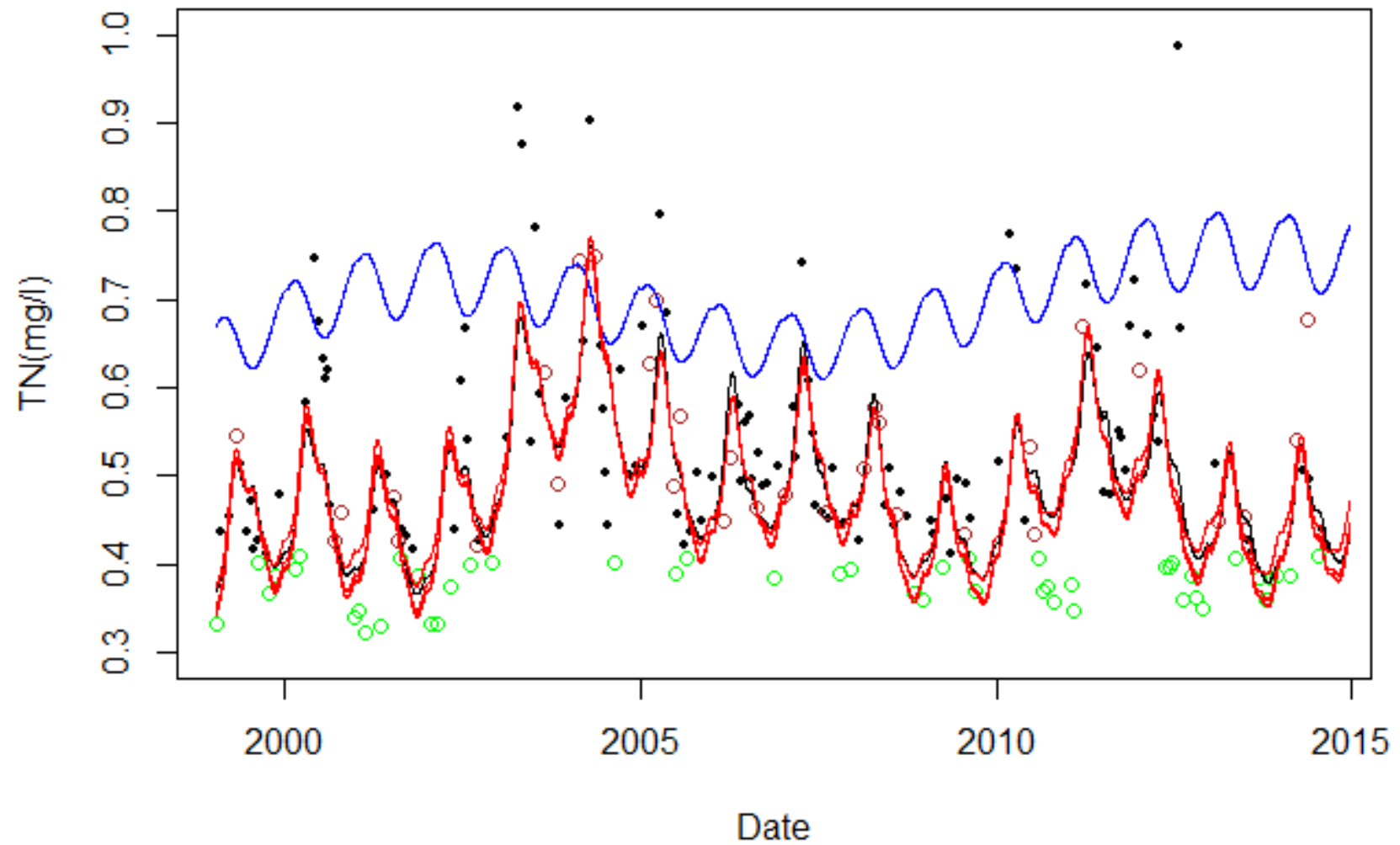


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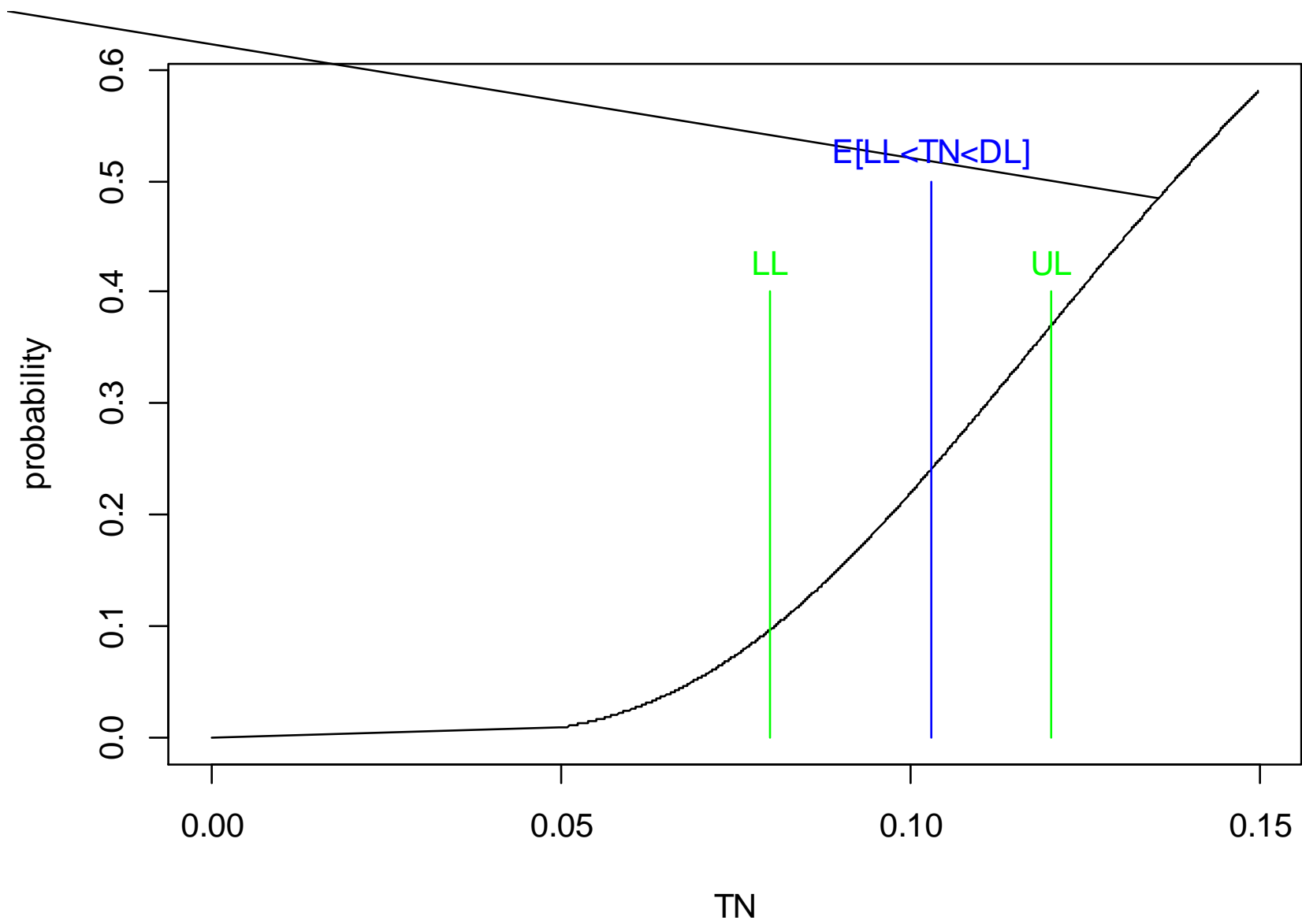


Substitute the expected value of the variable given that it is less than the

detection limit.

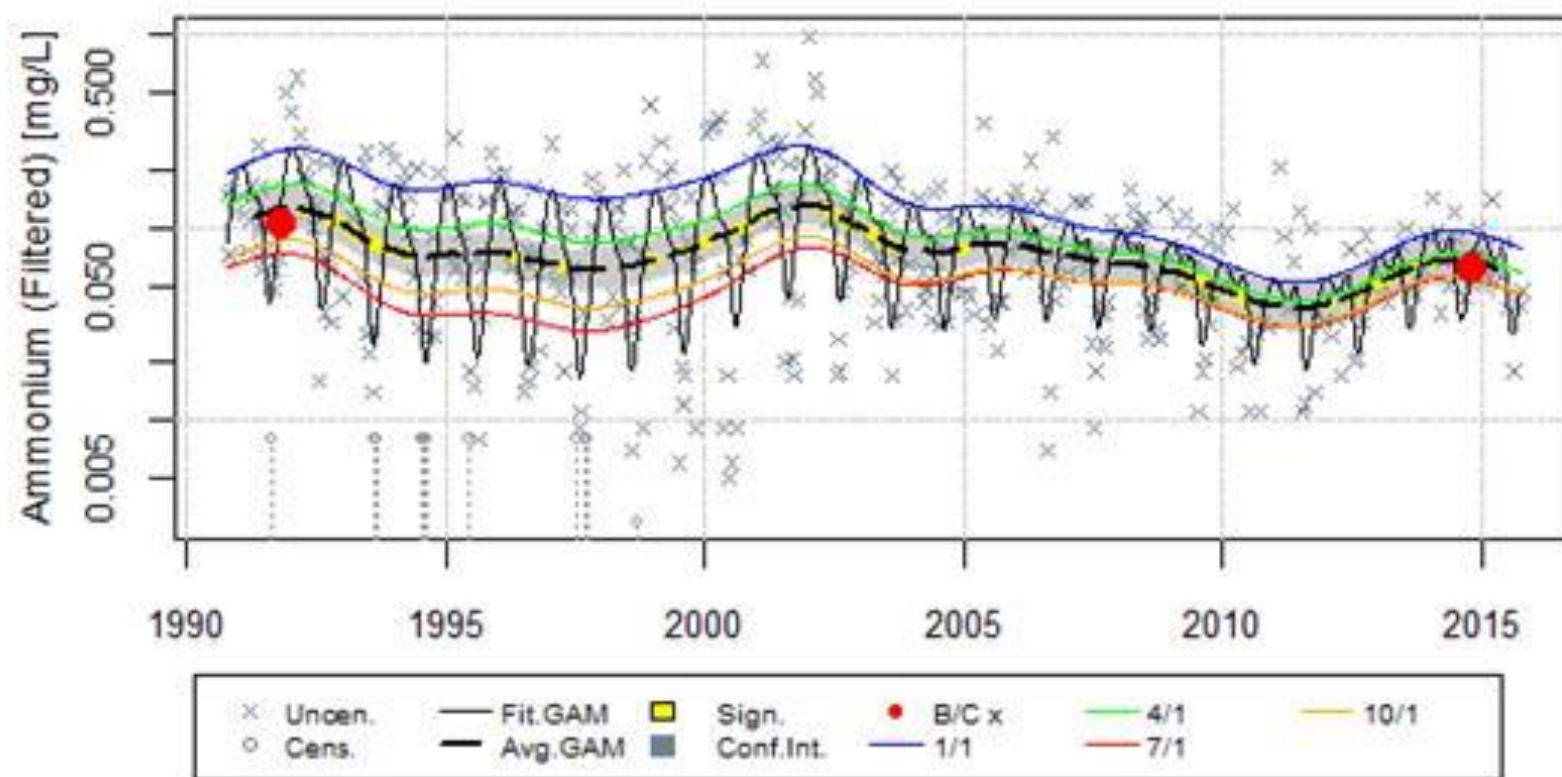


Convergence of EM algorithm.



Interval Censored Data.

Ammonium (Filtered)-Surface at TF2.2



Step Trend Models
(Intervention Models)
and
Methods Changes

Review old approach to methods changes

Review Maryland TSS case

Shows that Method Change effect can be unique to a station

Review issues with step trend model

Get your thoughts on this approach

Old Method:

Do a split sample study with multiple stations and dates.

Assess data with paired comparison test

Wilcoxon Signed Rank Test

Paired t-test

In cases of significant difference, estimate adjustment factor

Apply AF to old data to make is comparable to new.

(note: inherent assumption that the methods change effect is uniform
Over stations and dates)

Down the Road we found this

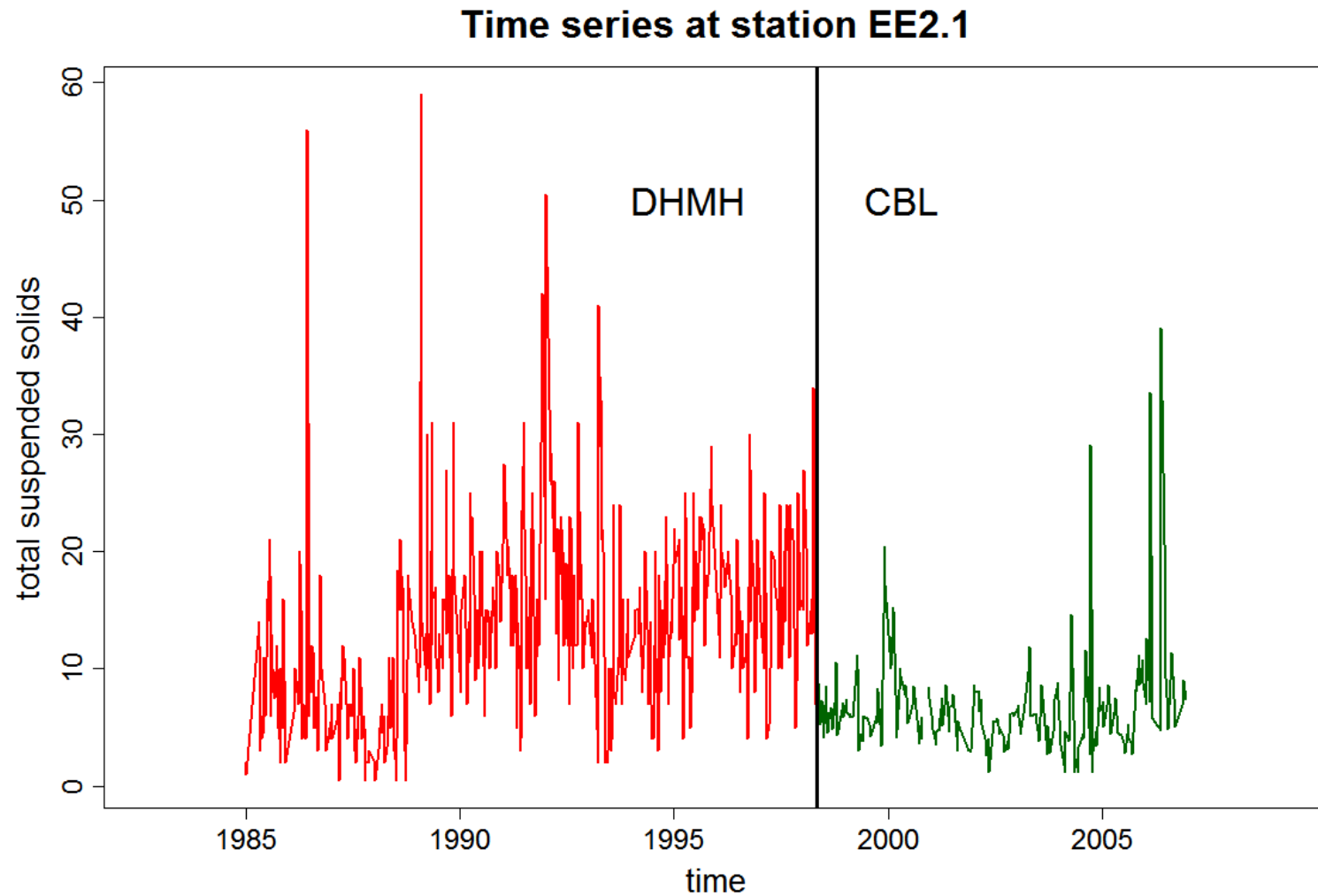


Figure 1. TSS at EE2.1(Choptank Embayment). The red curve shows data from DHMH. The green curve shows data from CBL. The black vertical line shows the point of laboratory change.

This effect was not consistent

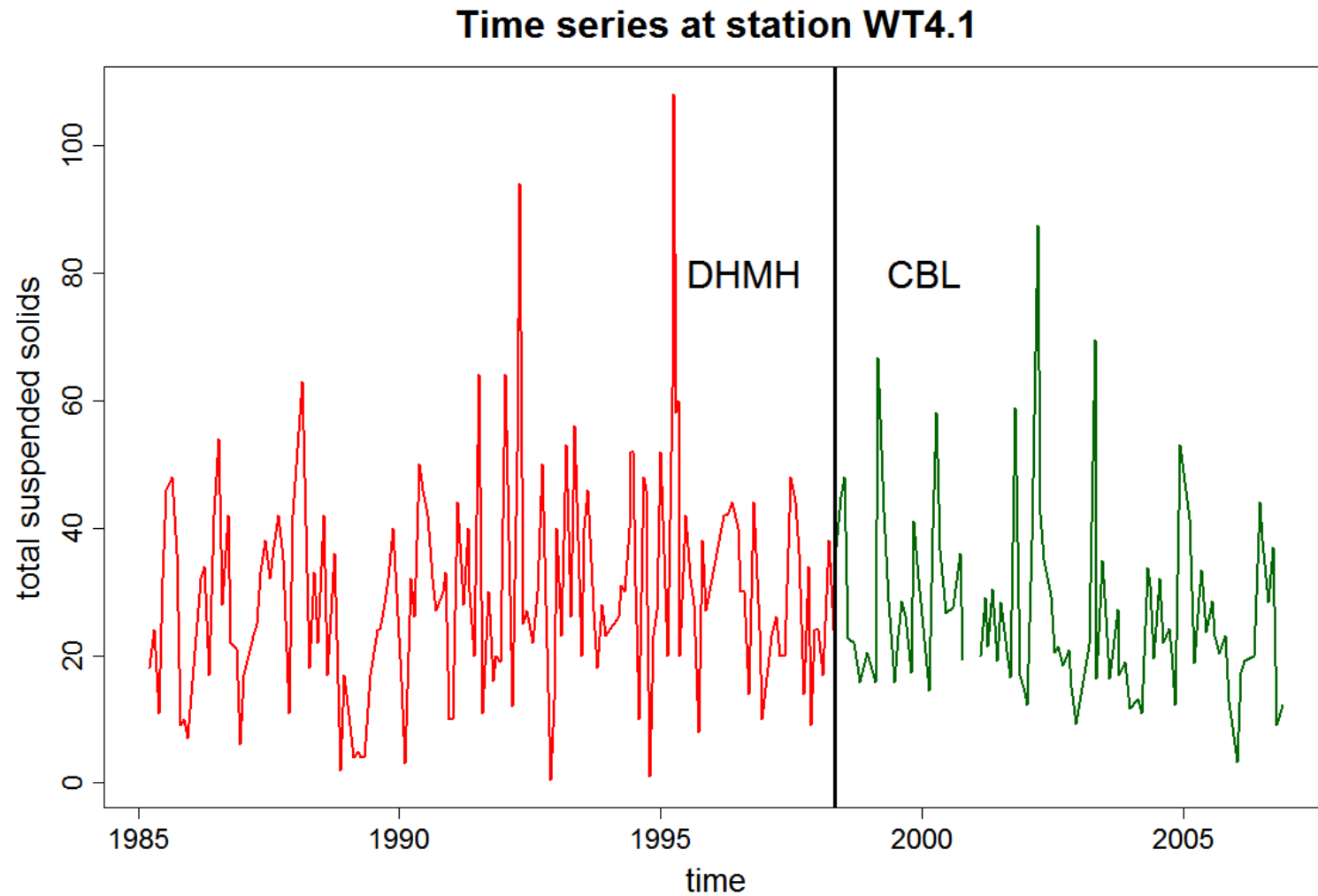
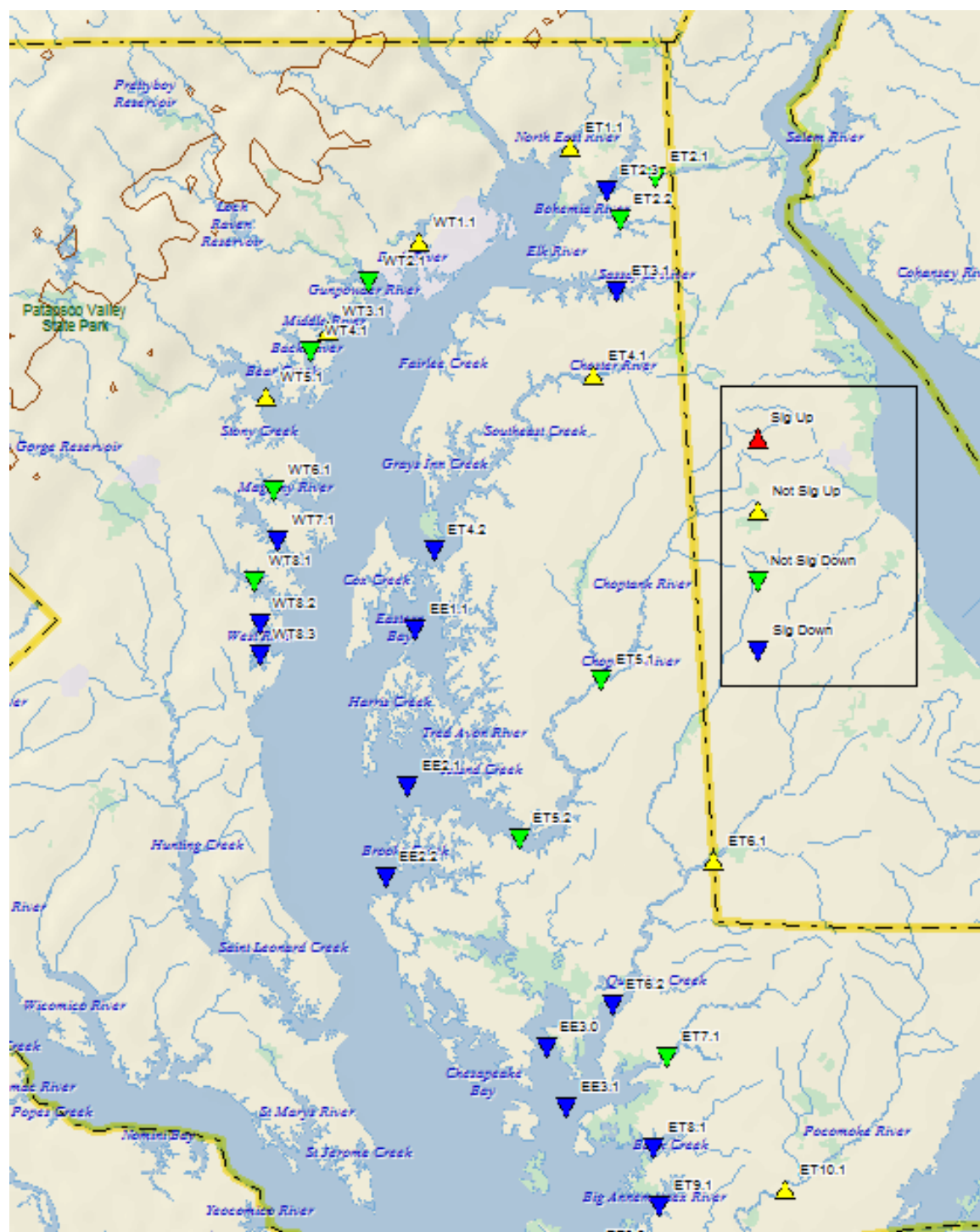


Figure 2. TSS at WT4.1 (Back River). The red curve shows data from DHMH. The green curve shows data from CBL. The black vertical line shows the point of laboratory change.



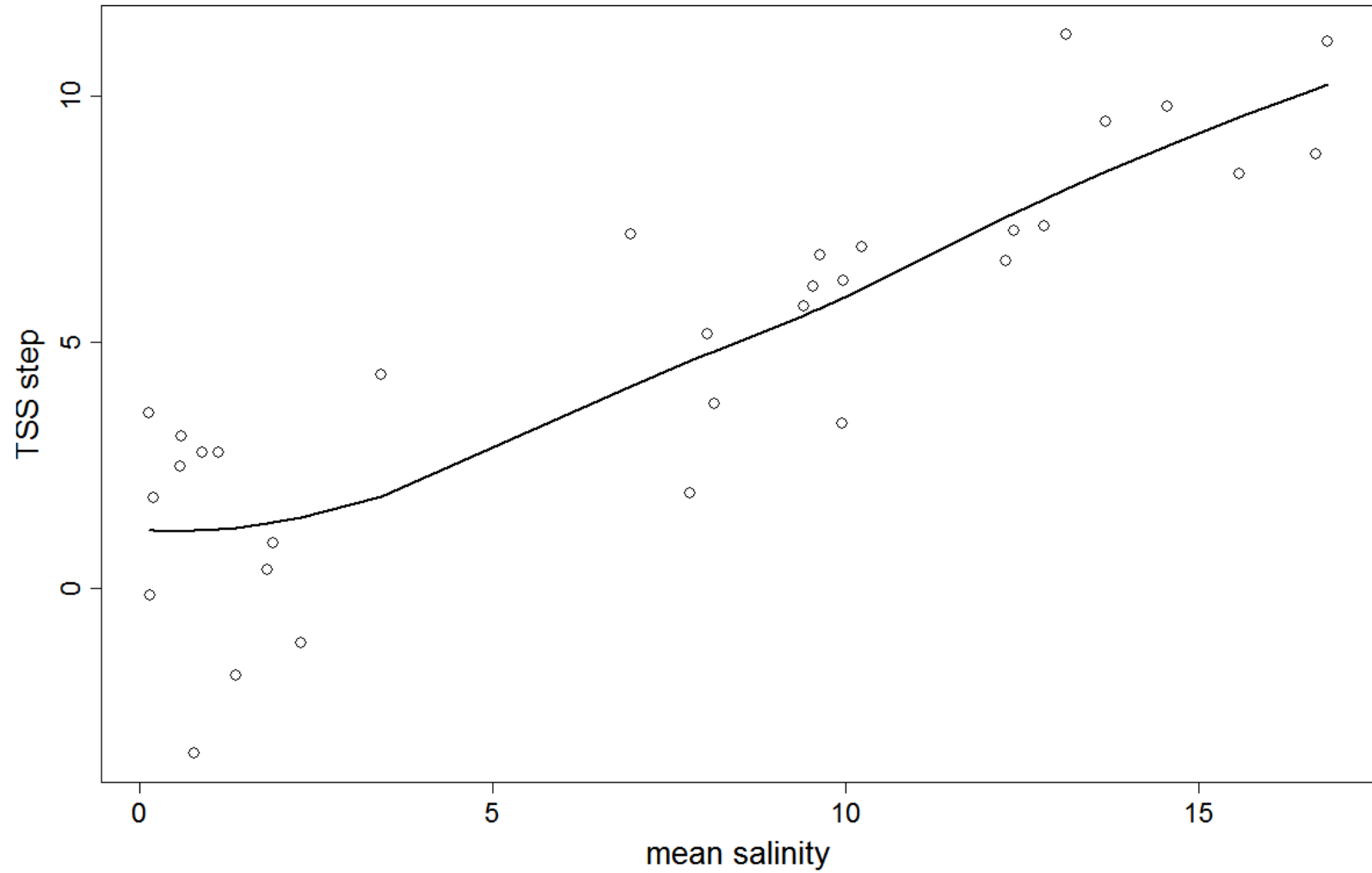
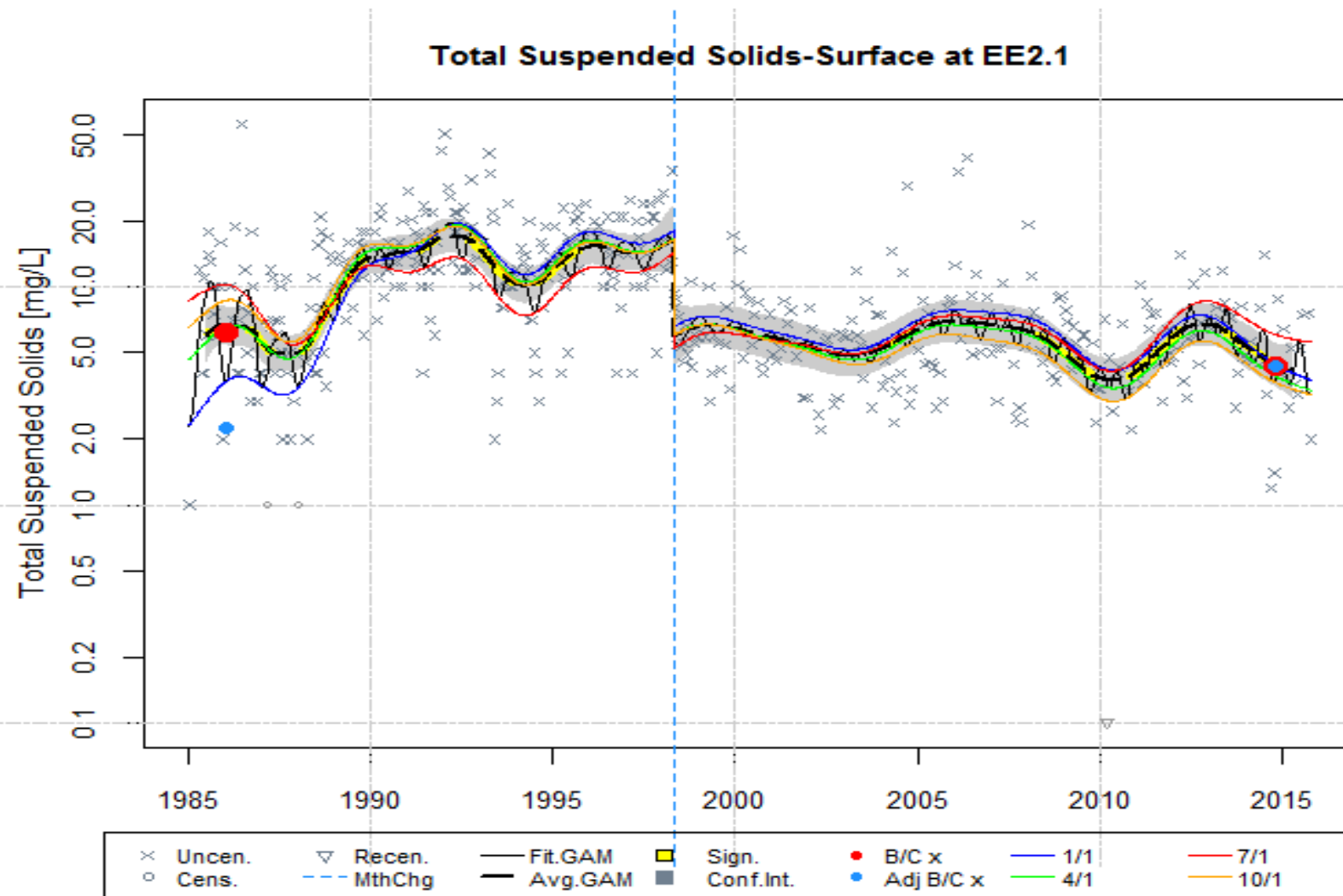
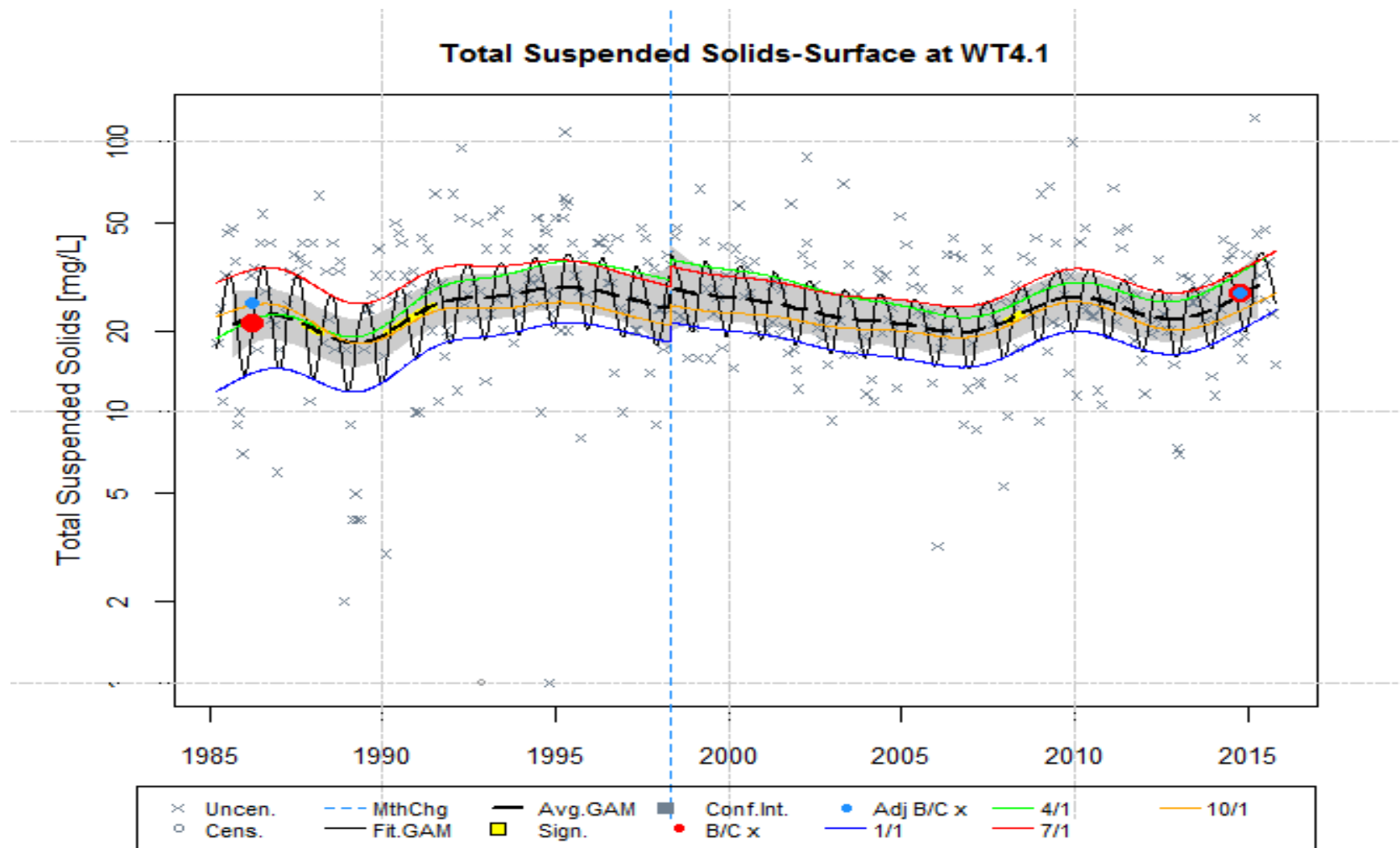


Figure 3. The TSS step size as a function of salinity for the 32 tributary stations. The fitted line is loess regression.



Baytrends model 3 fitted to EE2.1 (Choptank Embayment)TSS data.



Baytrends model 3 fitted to EE2.1 (Back River)TSS data.

This concludes the story that made us think we should develop a model that could assess Method Change effects station by station.

Now that we have it we have found other uses:

- a. BNR Assessment
- b. Dam Removal
- c. Catastrophic events (e.g. Agnes 1972)

We have also discovered some problems:

- a. 5 yrs pre and post
- b. Interventions close together cause problems
- c. A skip in the data with an intervention can lead to erroneous results
- d. Interventions that are confounded with natural events (e.g. flow change)

Engage the DIWG on two topics:

- a. Do you see issues with this approach to methods changes?
- b. If we find variable steps by station, will you help us assess the cause?

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