Regression Models - Morrison Bridge NAWQA

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Some info of Metolachlor:

Metolachlor is an herbicide used in agriculture to control grasses. Its use is controversial, the chemical is approved in the US for use, but NOT in the EU. There are tolerance levels for this chemical in agriculture, but no maximum allowable level in drinking water – only an advisory level. According to GHS (Globally Harmonized System for Hazard Communication), an international accord on chemical hazard, Metolachlor is:

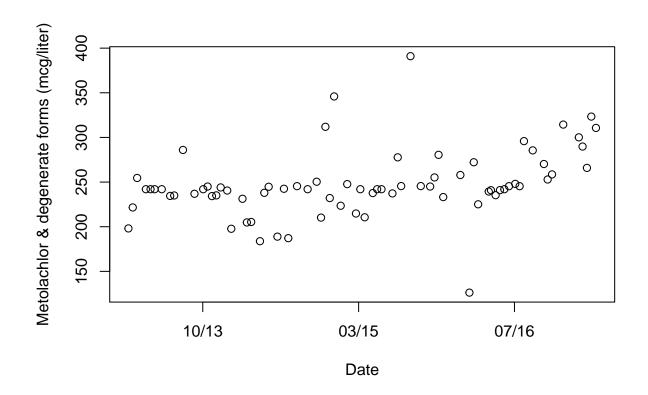
May cause an allergic skin reaction [Warning Sensitization, Skin - Category 1]

Fatal if inhaled [Danger Acute toxicity, inhalation - Category 1, 2]

Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard - Category 1]

Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard - Category 1]

```
plot(data.all$DateTime, data.all$metoforms, xlab = "Date", ylab = "Metolachlor & degenerate forms (mcg/
```



#lets try a simple general additive mixed model!
gam.meto<-gam(metoforms~Discharge+StreamVelocity+GageHeight+SensorDepth+WaterTemp+DissolvedO2+O2Saturat
summary(gam.meto)</pre>

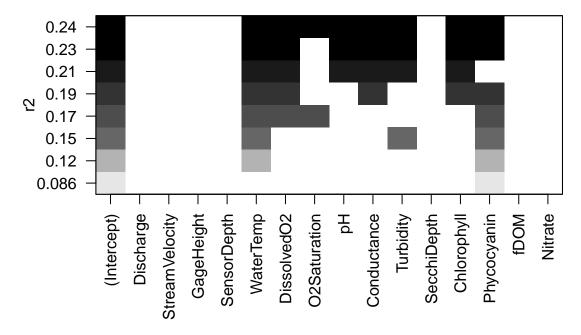
```
##
## Family: gaussian
## Link function: identity
##
## Formula:
   metoforms ~ Discharge + StreamVelocity + GageHeight + SensorDepth +
##
       WaterTemp + DissolvedO2 + O2Saturation + pH + Conductance +
       Turbidity + SecchiDepth + Chlorophyll + Phycocyanin + fDOM +
##
       Nitrate
##
##
## Parametric coefficients:
                    Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                   -735.5961
                               453.0750
                                         -1.624
                                                   0.1099
                                 3.0007
                                         -0.178
                                                   0.8591
## Discharge
                     -0.5350
## StreamVelocity
                     15.6134
                               116.5071
                                           0.134
                                                   0.8939
                     -5.0014
                                         -0.532
                                                   0.5968
## GageHeight
                                 9.4019
## SensorDepth
                      5.7730
                                 9.0040
                                           0.641
                                                   0.5239
                                           1.573
## WaterTemp
                     10.9407
                                 6.9564
                                                   0.1212
## Dissolved02
                     37.1763
                                           1.296
                                                   0.2002
                                28.6895
## 02Saturation
                     -1.7410
                                 2.6390
                                          -0.660
                                                   0.5120
                                           1.302
## pH
                     67.8281
                                52.0944
                                                   0.1981
## Conductance
                      1.5553
                                 0.9301
                                           1.672
                                                   0.0999 .
```

```
## Turbidity
                   1.7402
                              1.5456 1.126
                                              0.2648
                              4.4564 -0.873 0.3861
## SecchiDepth
                  -3.8917
## Chlorophyll
                              4.1103 -2.253 0.0280 *
                  -9.2617
## Phycocyanin
                  37.4974
                             33.4809
                                     1.120 0.2673
## fDOM
                  -0.4162
                              1.8511 -0.225
                                              0.8229
## Nitrate
                 -26.3492
                             40.4253 -0.652 0.5171
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
##
## R-sq.(adj) = 0.0658
                        Deviance explained = 25.8%
         1710 Scale est. = 1340.3
## GCV =
                                      n = 74
#reduced gam model, did a stepwise removal of factors with highest p-values
#If i remove any more than this, the % deviance explained drops drastically
reduced.gam.meto<-gam(metoforms~WaterTemp+DissolvedO2+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin,
summary(reduced.gam.meto)
##
## Family: gaussian
## Link function: identity
##
## Formula:
## metoforms ~ WaterTemp + DissolvedO2 + pH + Conductance + Turbidity +
      Chlorophyll + Phycocyanin
##
## Parametric coefficients:
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -590.2417 367.3369 -1.607 0.1129
                7.3345 3.5943 2.041 0.0453 *
## WaterTemp
## DissolvedO2 20.6528 12.3621 1.671 0.0995
## pH
              57.2329 39.2944 1.457 0.1500
## Conductance 1.1694 0.6158 1.899 0.0619
               1.4945
                          0.9118 1.639
## Turbidity
                                            0.1060
## Chlorophyll
              -7.9208
                           3.5383 -2.239
                                            0.0286 *
## Phycocyanin 31.1671
                          24.9213 1.251
                                           0.2155
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
##
## R-sq.(adj) = 0.146
                       Deviance explained = 22.8%
## GCV = 1374.2 Scale est. = 1225.7
#linear model
lm.meto<-lm(metoforms~Discharge+StreamVelocity+GageHeight+SensorDepth+WaterTemp+DissolvedO2+O2Saturation)
summary(lm.meto)
##
## lm(formula = metoforms ~ Discharge + StreamVelocity + GageHeight +
##
      SensorDepth + WaterTemp + DissolvedO2 + O2Saturation + pH +
      Conductance + Turbidity + SecchiDepth + Chlorophyll + Phycocyanin +
##
##
      fDOM + Nitrate, data = data.all)
##
## Residuals:
##
       Min
                 1Q
                                  30
                    Median
                                          Max
```

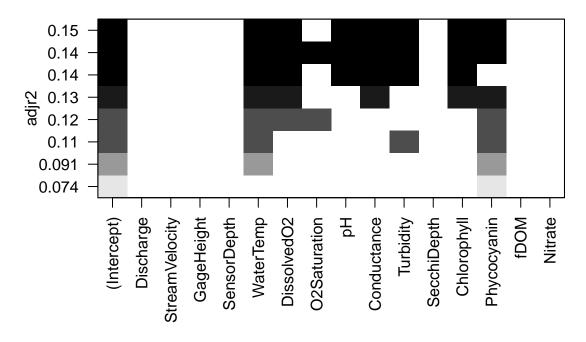
```
## -134.846 -14.244
                       2.444
                               10.521 108.683
##
## Coefficients:
##
                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                 -735.5961
                            453.0750 -1.624
                                                0.1099
## Discharge
                               3.0007 -0.178
                                                0.8591
                   -0.5350
## StreamVelocity
                                       0.134
                   15.6134 116.5071
                                                0.8939
                               9.4019 -0.532
## GageHeight
                   -5.0014
                                                0.5968
## SensorDepth
                    5.7730
                               9.0040
                                       0.641
                                                0.5239
## WaterTemp
                   10.9407
                              6.9564
                                       1.573
                                               0.1212
## Dissolved02
                   37.1763
                              28.6895
                                       1.296
                                               0.2002
## 02Saturation
                               2.6390 -0.660
                   -1.7410
                                               0.5120
## pH
                   67.8281
                              52.0944
                                       1.302
                                                0.1981
                                       1.672
                                                0.0999
## Conductance
                    1.5553
                            0.9301
                                       1.126
                                                0.2648
## Turbidity
                    1.7402
                              1.5456
## SecchiDepth
                   -3.8917
                               4.4564 -0.873
                                                0.3861
                               4.1103 -2.253
## Chlorophyll
                   -9.2617
                                                0.0280 *
## Phycocyanin
                   37.4974
                              33.4809
                                       1.120
                                                0.2673
                   -0.4162
                               1.8511 -0.225
                                                0.8229
## fDOM
## Nitrate
                  -26.3492
                              40.4253 -0.652
                                                0.5171
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 36.61 on 58 degrees of freedom
## Multiple R-squared: 0.2577, Adjusted R-squared: 0.06576
## F-statistic: 1.343 on 15 and 58 DF, p-value: 0.2078
reduced.lm<-lm(metoforms~WaterTemp+DissolvedO2+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin, data =
summary(reduced.lm)
##
## lm(formula = metoforms ~ WaterTemp + DissolvedO2 + pH + Conductance +
      Turbidity + Chlorophyll + Phycocyanin, data = data.all)
##
##
## Residuals:
##
       Min
                 1Q
                      Median
                                   3Q
                                           Max
## -131.063 -12.714
                      -1.717
                               13.474 104.427
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -590.2417
                          367.3369 -1.607
                                            0.1129
## WaterTemp
                 7.3345
                            3.5943
                                   2.041
                                             0.0453 *
## DissolvedO2
                20.6528
                           12.3621
                                   1.671
                                             0.0995
## pH
                57.2329
                           39.2944
                                    1.457
                                             0.1500
                                    1.899
## Conductance
                1.1694
                            0.6158
                                             0.0619 .
## Turbidity
                 1.4945
                            0.9118
                                    1.639
                                             0.1060
                -7.9208
                            3.5383 -2.239
                                             0.0286 *
## Chlorophyll
## Phycocyanin
                31.1671
                           24.9213
                                    1.251
                                             0.2155
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 35.01 on 66 degrees of freedom
## Multiple R-squared: 0.2276, Adjusted R-squared: 0.1456
## F-statistic: 2.778 on 7 and 66 DF, p-value: 0.01357
```

The linear model with all factors has only 'chlorophyll' as significant. Using the leaps package to test the optimal set of factors.

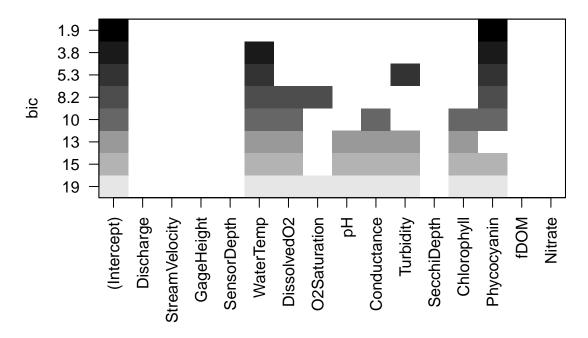
```
leaps.meto<-regsubsets(x = data.all[,4:18], y = data.all$metoforms)
plot(leaps.meto, scale = "r2")</pre>
```



plot(leaps.meto, scale = "adjr2")

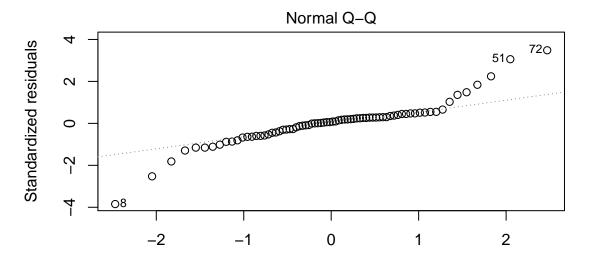


plot(leaps.meto, scale = "bic")



 $\begin{tabular}{ll} \#Now\ test\ for\ fit\ with\ these\ 3\ models\ created\ by\ leaps\\ \#full\ model \end{tabular}$

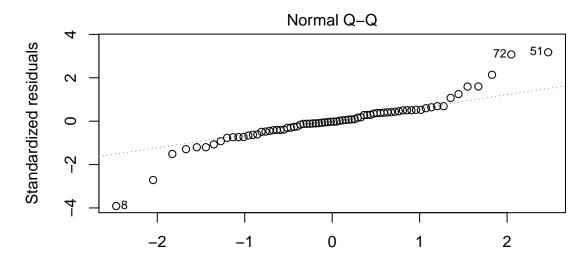
 $\verb|plot(lm(metoforms~Discharge+StreamVelocity+GageHeight+SensorDepth+WaterTemp+Dissolved02+02Saturation+pHissolved02+02Sa$



Theoretical Quantiles Im(metoforms ~ Discharge + StreamVelocity + GageHeight + SensorDepth + Wate .

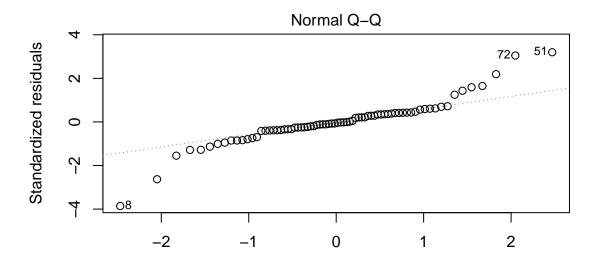
#highest r2

plot(lm(metoforms~WaterTemp+DissolvedO2+O2Saturation+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin,



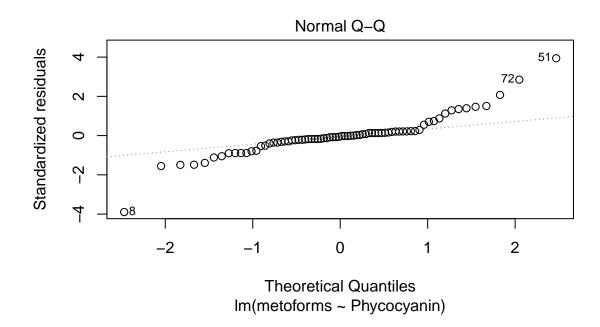
Theoretical Quantiles
Im(metoforms ~ WaterTemp + DissolvedO2 + O2Saturation + pH + Conductance + ...

#highest adjr2
plot(lm(metoforms~WaterTemp+DissolvedO2+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin, data = data.a



Theoretical Quantiles
Im(metoforms ~ WaterTemp + DissolvedO2 + pH + Conductance + Turbidity + Chl ...

```
#lowest BIC
plot(lm(metoforms~Phycocyanin, data = data.all), which = 2)
```



```
#quantile regression for meto with tau = .5
rq.meto<-rq(metoforms~WaterTemp+DissolvedO2+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin, data = da
summary(rq.meto)
##
  Call: rq(formula = metoforms ~ WaterTemp + DissolvedO2 + pH + Conductance +
##
       Turbidity + Chlorophyll + Phycocyanin, data = data.all)
##
## tau: [1] 0.5
##
## Coefficients:
               coefficients lower bd
                                       upper bd
## (Intercept) -285.12336
                            -983.40177
                                        323.35978
## WaterTemp
                  1.33968
                              -2.17665
                                           9.43410
## Dissolved02
                             -11.62171
                                          20.75141
                  0.77693
                 60.86486
                              -8.13841 110.82329
## pH
## Conductance
                  0.63455
                              -0.05009
                                          1.03935
                               0.03051
                                           2.38374
## Turbidity
                  1.70864
## Chlorophyll
                 -4.68017
                              -6.84272
                                           0.48336
## Phycocyanin
                 35.00731
                               1.45508
                                          85.75796
#Let's compare the AIC values for all of these models:
#AIC for quantile regression
AIC.rq(rq.meto)
## [1] 713.1188
## attr(,"edf")
```

```
## [1] 8
#AIC for full LM model
AIC(lm.meto)
## [1] 758.8205
#AIC for best linear model by BIC
AIC(lm(metoforms~Phycocyanin, data = data.all))
## [1] 746.2035
#AIC for best linear model by r2
AIC(lm(metoforms~WaterTemp+Dissolved02+02Saturation+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin, d
## [1] 746.8268
#AIC for best linear model by adjr2
AIC(lm(metoforms~WaterTemp+Dissolved02+pH+Conductance+Turbidity+Chlorophyll+Phycocyanin, data = data.al
## [1] 745.7691
#AIC for the two general additive mixed models
llgam<-logLik.gam(gam.meto)</pre>
AIC(llgam)
## [1] 758.8205
red.llgam<-logLik.gam(reduced.gam.meto)
AIC(red.llgam)
## [1] 745.7691
#nonlinear quantile regression estimate, havent got to work yet
\#nlrq.meto < -nlrq(metoforms \sim WaterTemp + Dissolved 02 + pH + Conductance + Turbidity + Chlorophyll + Phycocyanin, data
\verb|total<-data.all| \$ diaz forms + data.all| \$ meto forms + data.all| \$ hexaforms + data.all| \$ fip forms + data.all| \$ fip f
lm.all<-lm(total~Discharge+StreamVelocity+GageHeight+SensorDepth+WaterTemp+Dissolved02+02Saturation+pH+
summary(lm.all)
##
## Call:
## lm(formula = total ~ Discharge + StreamVelocity + GageHeight +
               SensorDepth + WaterTemp + DissolvedO2 + O2Saturation + pH +
##
               Conductance + Turbidity + SecchiDepth + Chlorophyll + Phycocyanin +
##
##
               fDOM + Nitrate, data = data.all)
##
## Residuals:
##
               Min
                                   1Q Median
                                                                        30
                                                                                        Max
## -136.00 -34.32 -10.10 27.45 246.89
##
## Coefficients:
##
                                             Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                                        -1853.5910 896.8906 -2.067
                                                                                                             0.0432 *
## Discharge
                                                 2.9646
                                                                        5.9401 0.499
                                                                                                                 0.6196
## StreamVelocity
                                             -69.9011
                                                                     230.6331 -0.303
                                                                                                                 0.7629
## GageHeight
                                                                      18.6117 -0.772
                                                                                                               0.4434
                                             -14.3647
## SensorDepth
                                              19.0579
                                                                   17.8240 1.069
                                                                                                                 0.2894
                                                                        13.7707
                                                                                              1.209
                                                                                                                 0.2317
```

0.810

0.4214

56.7927

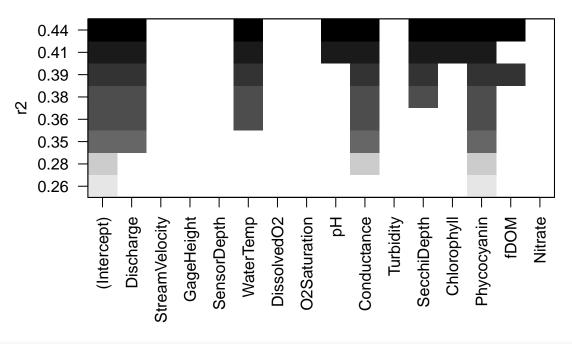
WaterTemp

Dissolved02

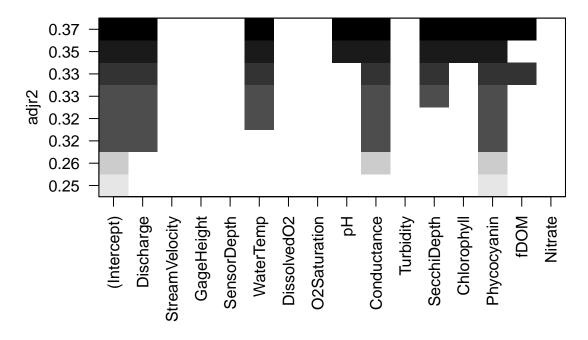
16.6452

45.9892

```
5.2240 -0.723
                                                   0.4724
## 02Saturation
                     -3.7784
## pH
                    258.2146
                               103.1242
                                           2.504
                                                   0.0151 *
## Conductance
                      4.1235
                                 1.8411
                                           2.240
                                                   0.0290 *
## Turbidity
                     -0.9972
                                 3.0596
                                         -0.326
                                                   0.7456
## SecchiDepth
                    -18.4593
                                 8.8217
                                         -2.092
                                                   0.0408 *
## Chlorophyll
                    -18.6846
                                 8.1367
                                         -2.296
                                                   0.0253 *
## Phycocyanin
                    145.6791
                                66.2776
                                          2.198
                                                   0.0320 *
## fDOM
                                 3.6645
                                                   0.0993 .
                     -6.1385
                                         -1.675
## Nitrate
                     89.3141
                                80.0245
                                           1.116
                                                   0.2690
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 72.47 on 58 degrees of freedom
## Multiple R-squared: 0.483, Adjusted R-squared: 0.3493
## F-statistic: 3.612 on 15 and 58 DF, p-value: 0.0002078
subset.all<-regsubsets(x = data.all[,4:18], y = total)</pre>
plot(subset.all, scale = "r2")
```



plot(subset.all, scale = "adjr2")



plot(subset.all, scale = "bic")

