ML interpolation

Amber Lee

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Load libraries

```
library(tidyverse)
library(stringr)
library(lubridate)

library(rpart) # for regression tree
library(rpart.plot)
library(caret) # for other models
library(rattle)
library(kableExtra)
library(broom)
```

Read data

```
water20 <- read.csv("cleaned_data.csv", header = TRUE)</pre>
```

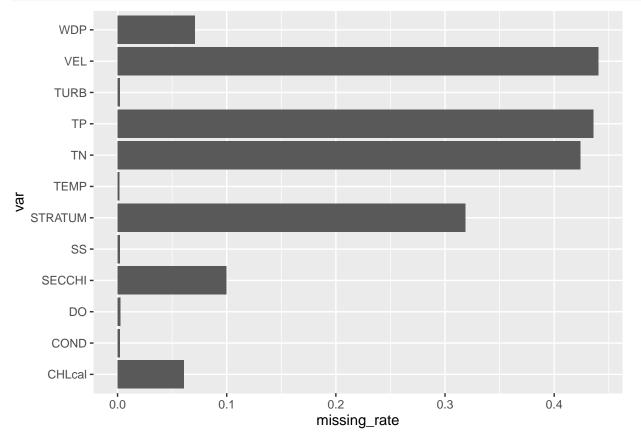
Very brief data exploration

Removed the QF code variable

Checked the missingness rate per variable

var	missing rate
VEL	0.440
TP	0.436
TN	0.424
STRATUM	0.319
SECCHI	0.100
WDP	0.071
CHLcal	0.061
DO	0.003
TEMP	0.002
TURB	0.002
COND	0.002
SS	0.002
SHEETBAR	0.000
DATE	0.000
LATITUDE	0.000
LONGITUDE	0.000
FLDNUM	0.000
LOCATCD	0.000
	·

```
var_missing_rate %>% filter(missing_rate > 0) %>%
ggplot(aes(x = var, y = missing_rate)) +
geom_bar(stat = "identity") +
coord_flip()
```



Added year and season variables, changed the FLDNUM variable to be categorical (character).

** I filtered out observations where TP was greater than 2 because that represented .1% of the data **

Notes

- regression (what are the steps for it?)
- classification and regression trees (CART)
- neural networks
- support vector machines

predicting TP with entire dataset

80/20

There are:

- 105,000 samples in the filtered water dataset water20
- 59,000 samples in the training data fullTP. This is because the testing and training data both need existing TP values
- 47,000 samples in the watertrain1
- and 11,800 samples in the watertest1

using the rpart library

```
https://www.statmethods.net/advstats/cart.html
```

```
tr.TP <- rpart(TP ~ .,</pre>
              data = watertrain1,
              control = rpart.control(xval = 15,
                                     minsplit = 100))
printcp(tr.TP)
##
## Regression tree:
## rpart(formula = TP ~ ., data = watertrain1, control = rpart.control(xval = 15,
      minsplit = 100))
##
##
## Variables actually used in tree construction:
## [1] COND SS
                TEMP TURB
## Root node error: 1252.8/47394 = 0.026434
##
## n= 47394
##
##
          CP nsplit rel error xerror
## 1 0.290222
                  0 1.00000 1.00003 0.022199
## 2 0.080946
                     0.70978 0.71062 0.019402
## 3 0.040385
                  2 0.62883 0.62947 0.017458
## 4 0.027189
                 3 0.58845 0.59008 0.016191
## 5 0.023035
                 4 0.56126 0.56303 0.015791
## 6 0.021124
                 5 0.53822 0.53991 0.015655
## 7 0.016767
                  6 0.51710 0.51915 0.015577
## 8 0.010873
                  7 0.50033 0.50647 0.015435
## 9 0.010000
                      0.48946 0.50134 0.015413
png("tree_TP.png")
fancyRpartPlot(tr.TP)
dev.off()
## pdf
png("tree_TP_CV.png")
plotcp(tr.TP)
dev.off()
## pdf
##
summary(tr.TP)
## Call:
## rpart(formula = TP ~ ., data = watertrain1, control = rpart.control(xval = 15,
      minsplit = 100))
##
    n = 47394
##
##
            CP nsplit rel error
                                               xstd
```

```
1 0.7097778 0.7106159 0.01940201
## 2 0.08094634
## 3 0.04038529
                     2 0.6288315 0.6294724 0.01745763
## 4 0.02718854
                     3 0.5884462 0.5900796 0.01619053
## 5 0.02303451
                     4 0.5612577 0.5630315 0.01579095
## 6 0.02112450
                     5 0.5382232 0.5399098 0.01565544
                     6 0.5170987 0.5191532 0.01557656
## 7 0.01676703
## 8 0.01087301
                     7 0.5003316 0.5064659 0.01543478
                     8 0.4894586 0.5013362 0.01541311
## 9 0.01000000
##
## Variable importance
        TURB
                          FLDNUM LATITUDE LONGITUDE
                                                           COND
                                                                   SECCHI
                                                                                TEMP
                    27
##
          39
                               7
                                          7
                                                              6
                                                                        6
##
## Node number 1: 47394 observations,
                                          complexity param=0.2902222
##
     mean=0.1964352, MSE=0.02643391
##
     left son=2 (33800 obs) right son=3 (13594 obs)
##
     Primary splits:
##
         TURB
                  < 38.5
                              to the left, improve=0.2895250, (105 missing)
##
         SECCHI
                  < 28.5
                              to the right, improve=0.2309235, (7909 missing)
                              to the left, improve=0.2290521, (159 missing)
##
                  < 37.39
##
         LATITUDE < 41.11549 to the right, improve=0.1822682, (0 missing)
##
                  splits as LRRRLL, improve=0.1808393, (557 missing)
##
     Surrogate splits:
                               to the left, agree=0.920, adj=0.721, (101 split)
##
         SS
                   < 46.805
##
         LATITUDE < 40.32079 to the right, agree=0.786, adj=0.251, (4 split)
##
                   splits as LLRRLL, agree=0.782, adj=0.241, (0 split)
##
         LONGITUDE < -89.72545 to the left, agree=0.778, adj=0.224, (0 split)
                               to the right, agree=0.773, adj=0.208, (0 split)
##
         SECCHI
                   < 28.5
##
## Node number 2: 33800 observations,
                                          complexity param=0.04038529
##
     mean=0.1408882, MSE=0.01081529
##
     left son=4 (32363 obs) right son=5 (1437 obs)
##
     Primary splits:
##
         COND
                              to the left, improve=0.13838440, (114 missing)
                  < 738.5
                  < 18.5
##
         TURB
                              to the left,
                                            improve=0.10829110, (60 missing)
##
                  splits as LRRLLL, improve=0.09726929, (532 missing)
         FLDNUM
##
         LATITUDE < 41.77794 to the right, improve=0.08999491, (0 missing)
##
         SECCHI
                  < 47.5
                              to the right, improve=0.08849416, (6260 missing)
##
## Node number 3: 13594 observations,
                                          complexity param=0.08094634
     mean=0.334547, MSE=0.03852133
##
     left son=6 (12888 obs) right son=7 (706 obs)
##
     Primary splits:
                              to the left, improve=0.19146020, (45 missing)
##
         TURB
                  < 307
##
         SS
                  < 584.65
                              to the left, improve=0.17680420, (54 missing)
                              to the right, improve=0.09771220, (1649 missing)
##
                  < 11.5
         SECCHI
                  splits as LLRLLR, improve=0.05577148, (25 missing)
##
##
         LATITUDE < 38.94276 to the left, improve=0.04493640, (0 missing)
##
     Surrogate splits:
##
         SS < 410.75
                        to the left, agree=0.975, adj=0.519, (41 split)
##
## Node number 4: 32363 observations,
                                          complexity param=0.0211245
##
    mean=0.1327355, MSE=0.00667315
     left son=8 (22056 obs) right son=9 (10307 obs)
```

1

```
##
     Primary splits:
##
         TURB
                            to the left, improve=0.12253150, (56 missing)
               < 17.5
         SECCHI < 47.5
##
                            to the right, improve=0.10193660, (5957 missing)
                            to the left, improve=0.09280021, (80 missing)
##
         TEMP
               < 21.35
##
                < 14.465
                            to the left, improve=0.09034200, (101 missing)
##
         DO
                            to the right, improve=0.08267267, (151 missing)
                < 8.45
##
     Surrogate splits:
                               to the left, agree=0.892, adj=0.662, (56 split)
##
         SS
                   < 21.81
         LATITUDE < 41.74147 to the right, agree=0.756, adj=0.233, (0 split)
##
##
                   splits as LRRRLL, agree=0.743, adj=0.193, (0 split)
         LONGITUDE < -90.11358 to the left, agree=0.714, adj=0.103, (0 split)
##
                               to the right, agree=0.709, adj=0.085, (0 split)
##
         SECCHI
                   < 47.5
##
## Node number 5: 1437 observations
##
     mean=0.3244962, MSE=0.0688925
##
## Node number 6: 12888 observations,
                                         complexity param=0.02718854
##
     mean=0.3143319, MSE=0.02699046
     left son=12 (10334 obs) right son=13 (2554 obs)
##
##
     Primary splits:
##
         COND
                  < 667.5
                              to the left, improve=0.09719369, (23 missing)
##
         FLDNUM
                  splits as LLRLLL, improve=0.08934998, (23 missing)
                              to the right, improve=0.06942041, (1493 missing)
##
                  < 16.5
         SECCHI
                              to the left, improve=0.06591051, (44 missing)
##
         TURB
                  < 101.5
##
         LATITUDE < 38.94067 to the left, improve=0.06457725, (0 missing)
##
     Surrogate splits:
##
         FLDNUM splits as LLRLLL, agree=0.848, adj=0.231, (20 split)
##
## Node number 7: 706 observations,
                                       complexity param=0.01676703
     mean=0.7035737, MSE=0.1053764
##
##
     left son=14 (563 obs) right son=15 (143 obs)
##
     Primary splits:
##
         SS
                   < 797.4
                               to the left, improve=0.2868661, (6 missing)
##
         TURB
                               to the left, improve=0.2838516, (1 missing)
                   < 571
##
         LATITUDE < 39.98717 to the left,
                                             improve=0.2068708, (0 missing)
##
         LONGITUDE < -89.52492 to the right, improve=0.2059435, (0 missing)
##
         FLDNUM
                   splits as RRRLRR, improve=0.1947993, (2 missing)
##
     Surrogate splits:
##
                               to the left, agree=0.903, adj=0.521, (6 split)
         TURB
                   < 710
##
         LATITUDE < 44.55795 to the left, agree=0.800, adj=0.014, (0 split)
##
         LONGITUDE < -92.45883 to the right, agree=0.800, adj=0.014, (0 split)
##
## Node number 8: 22056 observations,
                                         complexity param=0.01087301
##
     mean=0.113187, MSE=0.004892865
     left son=16 (15762 obs) right son=17 (6294 obs)
##
##
     Primary splits:
##
         TEMP
                 < 20.35
                             to the left, improve=0.12668110, (54 missing)
##
         DO
                             to the right, improve=0.11464010, (109 missing)
                 < 8.45
         quarter < 3.5
##
                             to the right, improve=0.06091910, (0 missing)
##
         TURB
                 < 6.5
                             to the left, improve=0.05681586, (37 missing)
##
                             to the left, improve=0.05059193, (70 missing)
         SS
                 < 5.09
##
     Surrogate splits:
##
         DO
                  < 8.45
                              to the right, agree=0.809, adj=0.332, (1 split)
         LATITUDE < 37.32416 to the right, agree=0.716, adj=0.006, (53 split)
##
```

```
##
                   TN
                                     < 0.4125
                                                               to the right, agree=0.714, adj=0.000, (0 split)
##
## Node number 9: 10307 observations
          mean=0.1745675, MSE=0.007915123
##
##
## Node number 12: 10334 observations,
                                                                                        complexity param=0.02303451
          mean=0.2887743, MSE=0.01979563
          left son=24 (7155 obs) right son=25 (3179 obs)
##
##
          Primary splits:
##
                   TURB
                                   < 101.5
                                                            to the left, improve=0.14081750, (41 missing)
##
                   SECCHI < 16.5
                                                            to the right, improve=0.12720390, (1335 missing)
                                                            to the left, improve=0.09944958, (34 missing)
##
                                    < 161.15
                   SS
##
                   CHLcal < 85.60527 to the left, improve=0.06410087, (901 missing)
                   STRATUM splits as LLRRLRL, improve=0.04379174, (5219 missing)
##
##
          Surrogate splits:
##
                   SS
                                        < 141.45
                                                                 to the left, agree=0.891, adj=0.645, (38 split)
##
                   SECCHI
                                        < 15.5
                                                                 to the right, agree=0.754, adj=0.203, (3 split)
##
                   LATITUDE < 37.03289 to the right, agree=0.692, adj=0.003, (0 split)
##
                   LONGITUDE < -89.36861 to the left, agree=0.692, adj=0.003, (0 split)
##
## Node number 13: 2554 observations
          mean=0.4177428, MSE=0.04276542
##
## Node number 14: 563 observations
          mean=0.6166412, MSE=0.06636302
##
## Node number 15: 143 observations
          mean=1.045832, MSE=0.1120805
##
##
## Node number 16: 15762 observations
##
          mean=0.09748293, MSE=0.00339507
##
## Node number 17: 6294 observations
          mean=0.1525145, MSE=0.006479527
##
##
## Node number 24: 7155 observations
##
          mean=0.2535504, MSE=0.01510136
##
## Node number 25: 3179 observations
          mean=0.3680532, MSE=0.02128343
# tidy(tr.TP) TODO
https://rstudio-pubs-static.s3.amazonaws.com/27179\_e64f0de316fc4f169d6ca300f18ee2aa.html. Annual of the control of the contr
# Prediction error rate in training data = Root node error * rel error * 100%
# Prediction error rate in cross-validation = Root node error * xerror * 100%
# Hence we want the cp value (with a simpler tree) that minimizes the xerror.
bestcp <- tr.TP$cptable[which.min(tr.TP$cptable[,"xerror"]),"CP"]</pre>
bestcp
```

[1] 0.01

```
tr.TP.prune <- prune(tr.TP, cp = bestcp)

data.frame(round(tr.TP.prune$cptable, digits = 3)) %>%
  kbl(booktabs = T)
```

CP	nsplit	rel.error	xerror	xstd
0.290	0	1.000	1.000	0.022
0.081	1	0.710	0.711	0.019
0.040	2	0.629	0.629	0.017
0.027	3	0.588	0.590	0.016
0.023	4	0.561	0.563	0.016
0.021	5	0.538	0.540	0.016
0.017	6	0.517	0.519	0.016
0.011	7	0.500	0.506	0.015
0.010	8	0.489	0.501	0.015

https://datascience.stackexchange.com/questions/31346/caret-and-rpart-does-caret-automatically-prune-rpart-trees

http://www.rdatamining.com/docs/regression-and-classification-with-regression-and-classification-and-classif

Model evaluation

```
watertrain1$TP.PREDICT <- predict(tr.TP, data = watertrain1)

watertrain1 <- watertrain1 %>%
    mutate(TP.SQ.ERROR = (TP - TP.PREDICT)^2)

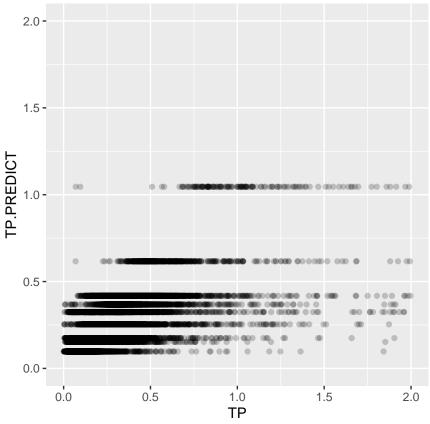
print("RSME is")

## [1] "RSME is"

sqrt(sum(watertrain1$TP.SQ.ERROR)/dim(watertrain1)[1])

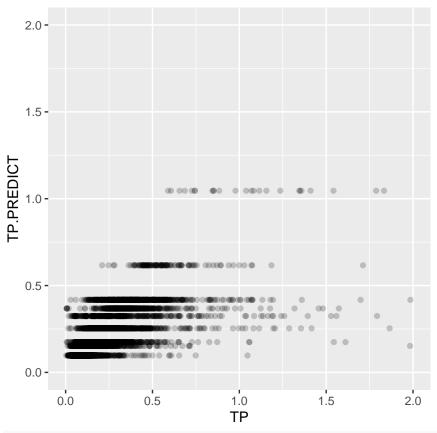
## [1] 0.1137467

watertrain1 %>%
    ggplot(aes(x = TP, y = TP.PREDICT)) +
    geom_point(alpha = 0.2) +
    coord_equal() +
    theme(aspect.ratio = 1) + xlim(0, 2) + ylim(0, 2)
```



```
ggsave("tree_training_predictvsactual.png")
watertest1$TP.PREDICT <- predict(tr.TP.prune, watertest1)
watertest1 <- watertest1 %>%
   mutate(TP.SQ.ERROR = (TP - TP.PREDICT)^2)
print("RSME is")
## [1] "RSME is"
sqrt(sum(watertest1$TP.SQ.ERROR)/dim(watertest1)[1])
## [1] 0.1120495
```

```
watertest1 %>%
  ggplot(aes(x = TP, y = TP.PREDICT)) +
  geom_point(alpha = 0.2) +
  coord_equal() +
  theme(aspect.ratio = 1) + xlim(0, 2) + ylim(0, 2)
```



ggsave("tree_test_predictvsactual.png")

```
watertrain2 <- fullTP[train_idx[,2],]
watertest2 <- fullTP[-train_idx[,2],]

# remove all na's because that's how GLM works
watertrain2 <- watertrain2 %>%
  filter_all(all_vars(!is.na(.)))
watertest2 <- watertest2 %>%
  filter_all(all_vars(!is.na(.)))

linreg <- glm(TP ~ ., data = watertrain2)
summary(linreg)</pre>
```

multivariate linear regression

```
##
## Call:
## glm(formula = TP ~ ., data = watertrain2)
##
## Deviance Residuals:
## Min 1Q Median 3Q Max
## -0.66410 -0.03954 -0.00907 0.02492 1.48913
##
## Coefficients:
```

```
##
                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                       2.784e+00 6.813e-01
                                            4.086 4.41e-05 ***
## LATITUDE
                      -8.436e-03 9.145e-03 -0.922 0.35629
## LONGITUDE
                                            4.092 4.29e-05 ***
                       2.661e-02 6.501e-03
## FLDNUMBrighton, IL -1.447e-02 2.925e-02
                                           -0.495 0.62090
## FLDNUMHavana, IL
                                            1.906 0.05663 .
                       3.452e-02 1.811e-02
## FLDNUMJackson, MO
                      -9.317e-02 4.357e-02 -2.139 0.03249 *
## FLDNUMLake City, MN 6.572e-02 2.331e-02
                                             2.819 0.00483 **
## FLDNUMOnalaska, WI
                       4.499e-02 1.587e-02
                                             2.834 0.00460 **
## STRATUM2
                       1.404e-03 3.816e-03
                                           0.368 0.71299
## STRATUM3
                       3.993e-03 4.072e-03
                                            0.981 0.32676
## STRATUM4
                       1.613e-01 7.570e-03 21.306 < 2e-16 ***
## STRATUM5
                      -8.705e-03 4.544e-03 -1.916 0.05544 .
                                            7.930 2.35e-15 ***
## STRATUM6
                       6.495e-02 8.190e-03
## STRATUM9
                      -1.816e-02 2.827e-02 -0.642 0.52071
## TN
                       4.787e-04 5.116e-04
                                             0.936 0.34947
## TEMP
                       2.061e-03 1.343e-04 15.353 < 2e-16 ***
## DO
                     -8.912e-03 3.194e-04 -27.902 < 2e-16 ***
## TURB
                      1.126e-03 4.109e-05 27.405 < 2e-16 ***
## COND
                       2.027e-04 9.164e-06 22.116 < 2e-16 ***
## VEL
                      -1.560e-03 2.682e-03 -0.582 0.56082
## SS
                      -2.453e-05 3.627e-05 -0.676 0.49891
## WDP
                      -2.772e-04 5.456e-04 -0.508 0.61140
## CHLcal
                      1.047e-03 3.281e-05 31.899
                                                    < 2e-16 ***
## SECCHI
                      -3.912e-04 3.000e-05 -13.039 < 2e-16 ***
## year
                      1.457e-05 1.125e-04
                                             0.130 0.89691
## quarter
                       1.672e-02 1.007e-03 16.599 < 2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for gaussian family taken to be 0.009330335)
##
##
      Null deviance: 320.12 on 14281 degrees of freedom
## Residual deviance: 133.01 on 14256 degrees of freedom
## AIC: -26202
## Number of Fisher Scoring iterations: 2
tidy(linreg) %>%
 filter(p.value < 0.05) %>%
 mutate(estimate = round(estimate, digits = 3),
        p.value = round(p.value, digits = 3)) %>%
 select(term, estimate, p.value) %>%
 kbl(booktabs = T)
```

term	estimate	p.value
(Intercept)	2.784	0.000
LONGITUDE	0.027	0.000
FLDNUMJackson, MO	-0.093	0.032
FLDNUMLake City, MN	0.066	0.005
FLDNUMOnalaska, WI	0.045	0.005
STRATUM4	0.161	0.000
STRATUM6	0.065	0.000
TEMP	0.002	0.000
DO	-0.009	0.000
TURB	0.001	0.000
COND	0.000	0.000
CHLcal	0.001	0.000
SECCHI	0.000	0.000
quarter	0.017	0.000

term	estimate	p.value
LATITUDE	-0.008	0.356
FLDNUMBrighton, IL	-0.014	0.621
FLDNUMHavana, IL	0.035	0.057
STRATUM2	0.001	0.713
STRATUM3	0.004	0.327
STRATUM5	-0.009	0.055
STRATUM9	-0.018	0.521
TN	0.000	0.349
VEL	-0.002	0.561
SS	0.000	0.499
WDP	0.000	0.611
year	0.000	0.897

mutate(TP.SQ.ERROR = (TP - TP.PREDICT)^2)

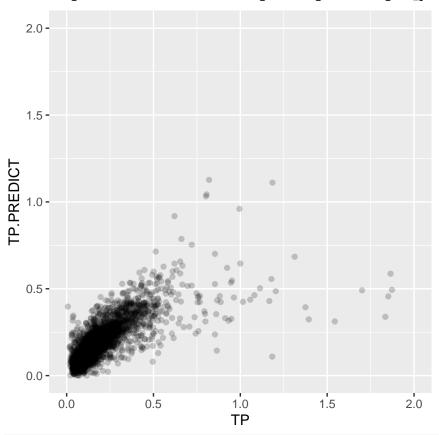
```
# watertrain2.selected <- fullTP[train_idx[,2],] %>%
# select(all_of(c("TEMP", "DO", "TURB", "COND", "FLDNUM",
# "CHLcal", "quarter"))) %>%
# filter_all(all_vars(!is.na(.)))
# TODO remove the missing values here and try to run the regression again, see if it applies to more value sum(fitted(linreg) == predict(linreg))
## [1] 14282
watertrain2$TP.PREDICT <- predict(linreg)</pre>
watertrain2 <- watertrain2 %>%
```

```
print("RSME is")
## [1] "RSME is"
sqrt(sum(watertrain2$TP.SQ.ERROR)/dim(watertrain2)[1])
## [1] 0.0965057
watertrain2 %>%
  ggplot(aes(x = TP, y = TP.PREDICT)) +
  geom_point(alpha = 0.2) +
  coord_equal() +
  theme(aspect.ratio = 1) + xlim(0, 2) + ylim(0, 2)
## Warning: Removed 32 rows containing missing values (geom_point).
   2.0 -
   1.5 -
TP.PREDICT
   1.0 -
   0.5 -
   0.0 -
        0.0
                     0.5
                                  1.0
                                                1.5
                                                             2.0
                                  ΤP
ggsave("glm_train_predictvsactual.png")
## Warning: Removed 32 rows containing missing values (geom_point).
watertest2$TP.PREDICT <- predict(linreg, watertest2)</pre>
watertest2 <- watertest2 %>%
  mutate(TP.SQ.ERROR = (TP - TP.PREDICT)^2)
print("RSME is")
```

[1] "RSME is"

```
sqrt(sum(watertest2$TP.SQ.ERROR)/dim(watertest2)[1])
## [1] 0.1048744
watertest2 %>%
    ggplot(aes(x = TP, y = TP.PREDICT)) +
    geom_point(alpha = 0.2) +
    coord_equal() +
    theme(aspect.ratio = 1) + xlim(0, 2) + ylim(0, 2)
```

Warning: Removed 9 rows containing missing values (geom_point).



```
ggsave("glm_test_predictvsactual.png")
```

Warning: Removed 9 rows containing missing values (geom_point).

TP by year and season

```
make_year_touples <- function(index, year_partition){
    # index goes from 1 to length(year_partition) - 1

return(c(year_partition[index], year_partition[index+1]))
}

tree_by_years <- function(year_touple, water_data){</pre>
```

```
# filter for specific group of years
  water_data <- water_data %>% filter(year >= year_touple[1] &
                                          year <= year_touple[2])</pre>
  fitControl <- caret::trainControl(method="cv")</pre>
 tr.TP <- caret::train(TP ~ .,</pre>
                         data = water_data,
                         # what is method?
                         method = "rpart2",
                         trControl = fitControl,
                         # don't quite understand maxdepth
                         tuneGrid = data.frame(maxdepth=1:20))
 return(tr.TP)
}
tree_by_season <- function(season, min_year, max_year, year_interval, water_data){</pre>
  # season can be 1, 2, 3, 4 with 1 being spring
  ## this is already processed in line 70
 year_partition <- seq(min_year, max_year, year_interval)</pre>
  # make a list of each year interval
  year_touples <- lapply(1:(length(year_partition)-1), make_year_touples, year_partition)</pre>
  water_data <- water_data %>% filter(quarter == season)
  tree_models <- lapply(year_touples, tree_by_years, water_data)</pre>
 return(tree_models)
```

TP spring

TP summer

TP fall

TP winter