CMDA-4654

Project 1

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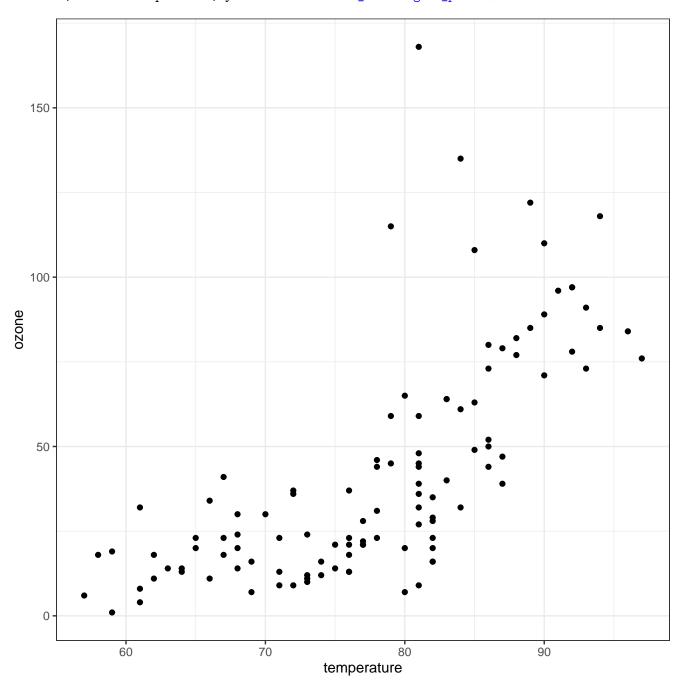
10/31/2021

Problem 1

```
library(dplyr)
library(ggplot2)

#setwd("C:/Users/Spencer/Downloads")
load("ozone.RData")

ggplot(ozone, aes(x = temperature, y = ozone)) + theme_bw() + geom_point()
```



Part a

Fitting polynomials of different degrees

```
model1 <- lm(ozone ~ poly(radiation,1), data = ozone)
model2 <- lm(ozone ~ poly(radiation,2), data = ozone)
model3 <- lm(ozone ~ poly(radiation,3), data = ozone)
model4 <- lm(ozone ~ poly(radiation,4), data = ozone)</pre>
```

```
model5 <- lm(ozone ~ poly(radiation,5), data = ozone)</pre>
model6 <- lm(ozone ~ poly(radiation,6), data = ozone)</pre>
summary(model1)
Call:
lm(formula = ozone ~ poly(radiation, 1), data = ozone)
Residuals:
   Min
             1Q Median
                             3Q
                                   Max
-48.292 -21.361 -8.864 16.373 119.136
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)
                    42.099
                                2.974 14.15 < 2e-16 ***
poly(radiation, 1) 121.572
                               31.335 3.88 0.000179 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 31.33 on 109 degrees of freedom
Multiple R-squared: 0.1213,
                               Adjusted R-squared: 0.1133
F-statistic: 15.05 on 1 and 109 DF, p-value: 0.0001793
summary(model2)
Call:
lm(formula = ozone ~ poly(radiation, 2), data = ozone)
Residuals:
    Min
             1Q Median
                             3Q
-40.155 -22.793 -6.438 18.061 115.117
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)
                     42.099
                                 2.832 14.864 < 2e-16 ***
poly(radiation, 2)1 121.572
                                 29.840 4.074 8.84e-05 ***
poly(radiation, 2)2 -104.178
                                29.840 -3.491 0.000698 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 29.84 on 108 degrees of freedom
Multiple R-squared: 0.2104,
                               Adjusted R-squared: 0.1958
F-statistic: 14.39 on 2 and 108 DF, p-value: 2.875e-06
summary(model3)
Call:
lm(formula = ozone ~ poly(radiation, 3), data = ozone)
Residuals:
          1Q Median
                        3Q
-45.05 -19.44 -4.52 15.61 109.95
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
                                 2.78 15.141 < 2e-16 ***
(Intercept)
                      42.10
                                 29.29 4.150 6.69e-05 ***
poly(radiation, 3)1 121.57
poly(radiation, 3)2 -104.18
                                 29.29 -3.556 0.000562 ***
poly(radiation, 3)3
                     -65.93
                                 29.29 -2.251 0.026450 *
```

```
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Residual standard error: 29.29 on 107 degrees of freedom
Multiple R-squared: 0.2461, Adjusted R-squared: 0.225
F-statistic: 11.65 on 3 and 107 DF, p-value: 1.154e-06
summary(model4)
Call:
lm(formula = ozone ~ poly(radiation, 4), data = ozone)
Residuals:
   Min
            1Q Median
                            3Q
                                  Max
-44.929 -19.519 -4.647 15.700 110.071
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
                                2.793 15.072 < 2e-16 ***
(Intercept)
                     42.099
poly(radiation, 4)1 121.572
                               29.428 4.131 7.23e-05 ***
poly(radiation, 4)2 -104.178
                               29.428 -3.540 0.000596 ***
poly(radiation, 4)3 -65.932
                                29.428 -2.240 0.027149 *
poly(radiation, 4)4
                      4.777
                               29.428 0.162 0.871356
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Residual standard error: 29.43 on 106 degrees of freedom
Multiple R-squared: 0.2463,
                              Adjusted R-squared: 0.2179
F-statistic: 8.661 on 4 and 106 DF, p-value: 4.352e-06
summary(model5)
Call:
lm(formula = ozone ~ poly(radiation, 5), data = ozone)
Residuals:
   Min
            1Q Median
                            3Q
                                  Max
-46.076 -16.978 -5.621 16.472 108.924
Coefficients:
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)
                     42.099 2.801 15.029 < 2e-16 ***
poly(radiation, 5)1 121.572
                               29.511 4.119 7.59e-05 ***
poly(radiation, 5)2 -104.178
                               29.511 -3.530 0.000618 ***
poly(radiation, 5)3 -65.932
                                29.511 -2.234 0.027595 *
                     4.777
                                29.511 0.162 0.871718
poly(radiation, 5)4
                     18.759
                                29.511 0.636 0.526389
poly(radiation, 5)5
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 29.51 on 105 degrees of freedom
Multiple R-squared: 0.2492,
                              Adjusted R-squared: 0.2135
F-statistic: 6.971 on 5 and 105 DF, p-value: 1.168e-05
summary(model6)
lm(formula = ozone ~ poly(radiation, 6), data = ozone)
Residuals:
```

```
1Q Median
                             3Q
    Min
                                    Max
-45.079 -17.204 -5.404 16.483 109.921
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)
                     42.099 2.812 14.971 < 2e-16 ***
poly(radiation, 6)1 121.572
                                 29.626 4.104 8.11e-05 ***
poly(radiation, 6)2 -104.178
                                 29.626 -3.516 0.00065 ***
poly(radiation, 6)3 -65.932 29.626 -2.225 0.02821 *
                     4.777
                                 29.626 0.161 0.87221
poly(radiation, 6)4
                    18.759
                                 29.626 0.633 0.52800
poly(radiation, 6)5
                                 29.626 -0.434 0.66527
poly(radiation, 6)6 -12.854
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 29.63 on 104 degrees of freedom
Multiple R-squared: 0.2506,
                                Adjusted R-squared: 0.2073
F-statistic: 5.795 on 6 and 104 DF, p-value: 3.079e-05
The polynomial fit that appears to work the best is the one with degree 3.
Part b
Writing the function that carries out LOESS regression
# This function has the following inputs.
#
# * x - a numeric input vector
# * y - a numeric response
# Note span and degree are shown with their default values.
# * degree should be 1 or 2 only
# * span can be any value in interval (0, 1) non-inclusive.
# If show.plot = TRUE then a plot of the final fit is shown
myloess <- function(x, y, span = 0.5, degree = 1, show.plot = TRUE) {
  # Getting range of values
  xrange <- diff(range(x))</pre>
  # Checking span meets requirements and setting width
  if (between(span, 0, 1)) {
    width <- span*xrange
    stop("Span must be between 0 and 1 non-inclusive")
  # Getting total number of points and windows (they'll be the same)
  N_total <- length(x)</pre>
  Win_total <- length(x)
  # Allocating space for vector of each window's population
  n_points <- vector(mode = "integer", length = length(x))</pre>
  # Allocating space for vector of fitted values
  yhat <- vector(mode = "numeric", length = length(x))</pre>
```

Combining our variables in data frame

mydata <- cbind.data.frame(x, y)</pre>

```
# Fitting each point
for(x0 in x) {
  # Setting population of window
  sample <- subset(mydata, between(x, x0-width/2, x0+width/2))</pre>
  n <- length(sample[,1])</pre>
  # Getting weights into diagonal matrix
  weights <- (1-(abs(sample[,1] - x0)/width*2)^3)^3
  W_mat <- diag(weights, n, n)</pre>
  # Checking degree and completing our regression accordingly
  if (degree == 1) {
    X_mat <- cbind(rep(1, n), sample[,1])</pre>
    betahat <- solve( t(X_mat)%*%W_mat%*%X_mat ) %*% t(X_mat) %*% W_mat %*% sample[,2]
    # Getting fitted value
    yhat[which(x0 == x)] \leftarrow betahat[1] + betahat[2]*x0
  }
  else if (degree == 2) {
    X_mat <- cbind(rep(1, n), sample[,1], sample[,1]^2)</pre>
    betahat <- solve( t(X_mat)%*%W_mat%*%X_mat ) %*% t(X_mat) %*% W_mat %*% sample[,2]
    # Getting fitted value
    yhat[which(x0 == x)] \leftarrow betahat[1] + betahat[2]*x0 + betahat[3]*x0^2
  }
  else {
    stop("Degree must be set to either 1 or 2")
  # Getting population of window
  n_{points[which(x0 == x)] <- n}
# Calculating SSE, MSE, and residual standard error
SSE <- sum((y-yhat)^{2})</pre>
MSE <- SSE/(N total-2)
RSE <- sqrt(MSE)</pre>
# Creating plot of final fit
loessplot <- ggplot(mydata, aes(x, y)) +</pre>
  geom_point(size = 3, alpha = 0.5, color = "grey") +
  geom_line(aes(x, yhat), color = "red", lty = 1) +
  xlab(deparse(substitute(x))) + ylab(deparse(substitute(y))) +
  ggtitle(paste("LOESS with degree =", degree, "and span =", span, sep = " "))
# Checking whether to show plot or not
if (show.plot == T) {
  print(loessplot)
}
# Returning named list
return(invisible(list(span = span, degree = degree, N_total = N_total, Win_total = Win_total,
            n_points = n_points, SSE = SSE, RSE = RSE, loessplot = loessplot)))
```

Determining LOESS regression fits on the data

}

```
# Creating an empty data frame
fit_table <- data.frame()</pre>
# Determining fits and putting info into data frame
for(j in 1:2) {
  for (i in seq(0.25, 0.75, by = 0.05)) {
    fit_table <- rbind(fit_table, c(i, j, myloess(ozone$temperature, ozone$ozone,</pre>
                                                  span = i, degree = j, show.plot = F)$RSE))
}
# Changing column names
colnames(fit_table) <- c("Span", "Degree", "RSE")</pre>
# Displaying data frame
fit_table
   Span Degree
                    RSE
1 0.25
            1 21.69723
2 0.30
            1 21.84914
3 0.35
           1 21.87405
4 0.40
          1 21.87005
5 0.45
           1 21.88484
          1 21.92533
6 0.50
7 0.55
           1 21.98316
           1 22.05339
8 0.60
        1 22.12531
1 22.18786
9 0.65
10 0.70
           1 22.24218
11 0.75
           2 20.70123
12 0.25
           2 21.21788
13 0.30
          2 21.65352
14 0.35
15 0.40
           2 21.83486
           2 21.82088
16 0.45
17 0.50
            2 21.75230
18 0.55
           2 21.71153
19 0.60
           2 21.71786
           2 21.76031
20 0.65
21 0.70
            2 21.81288
             2 21.86516
22 0.75
```

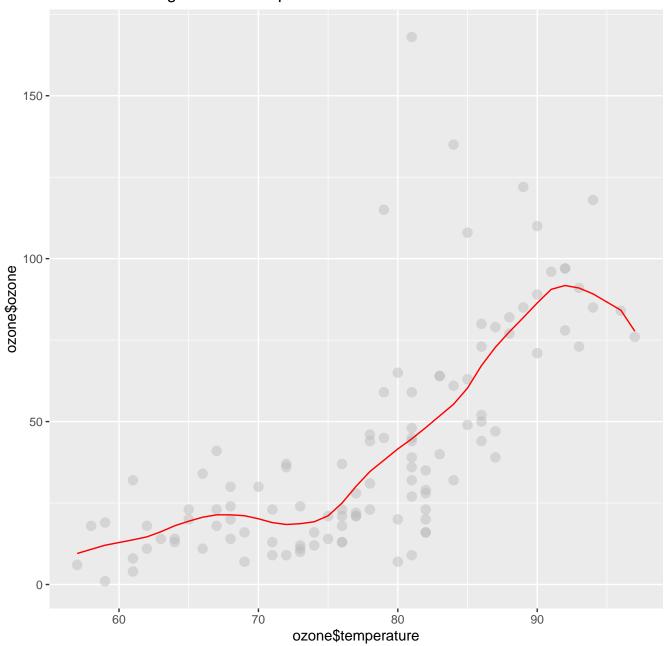
The three "best" fits with degree 1 appear to be span 0.25, 0.30, and 0.40. The three "best" fits with degree 2 appear to be span 0.25, 0.30, and 0.35.

Plotting the best fits found above

```
myloess(ozone$temperature, ozone$ozone,
```

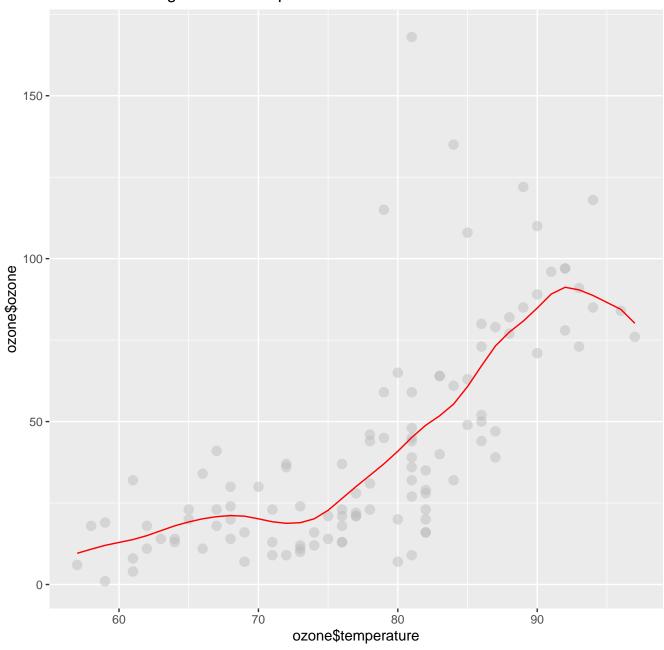
span = 0.25, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.25



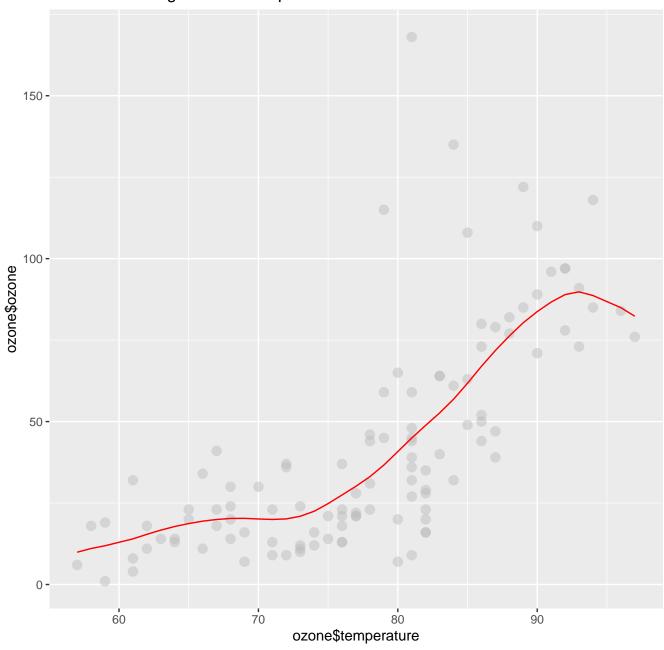
span = 0.30, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.3



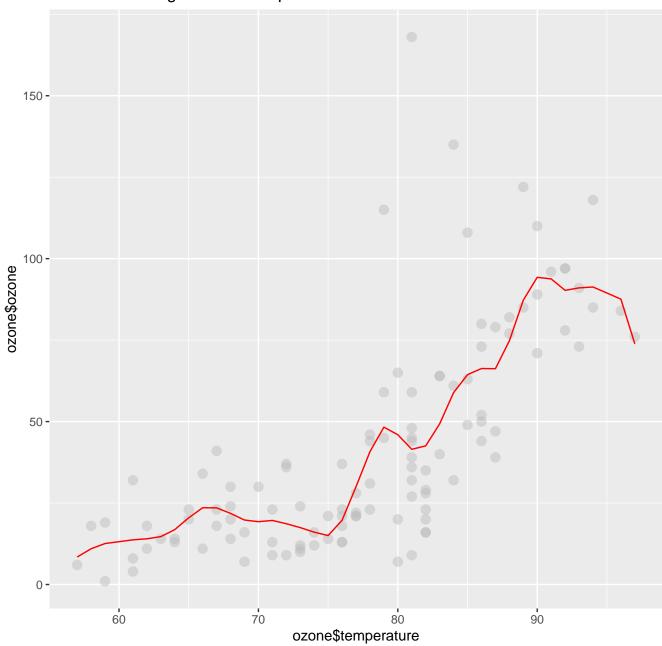
span = 0.40, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.4



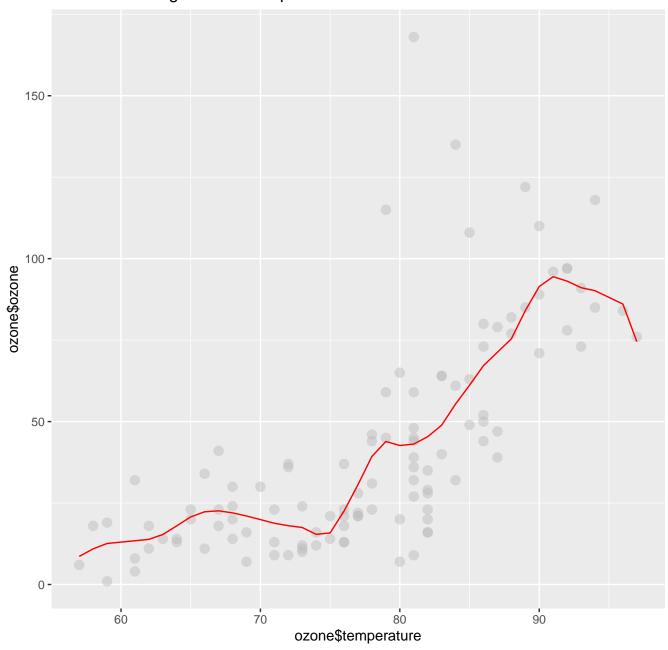
span = 0.25, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.25



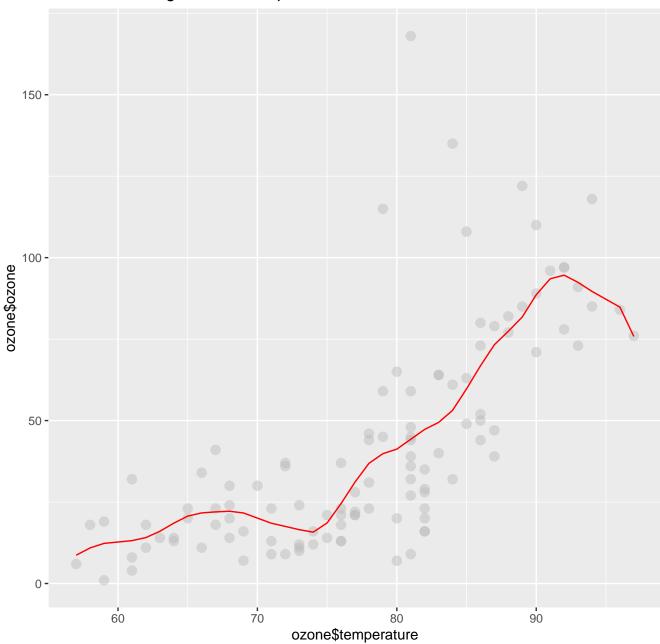
span = 0.30, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.3



span = 0.35, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.35

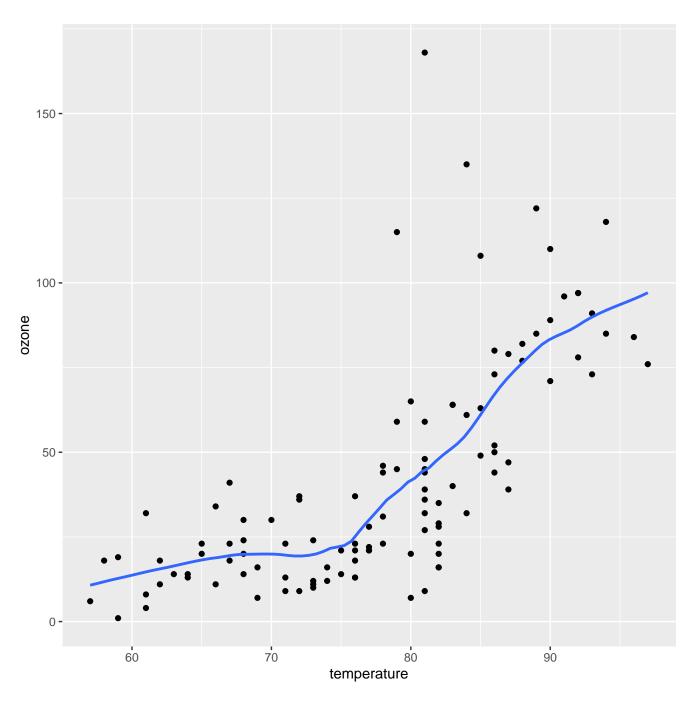


Visually inspecting the best fits compared to the 2nd and 3rd best fits, we do feel we may have over-fit the data, especially for the fits with degree 2. The model with degree 1 and span 0.4 appears to be the "best" fit.

Part c

```
Comparing results with built-in LOESS function \,
```

```
ozone %>% ggplot(aes(temperature, ozone)) +
  geom_point() +
  geom_smooth(method = "loess", degree = 1, span = 0.40, se = F, method.args = list(degree=1))
```

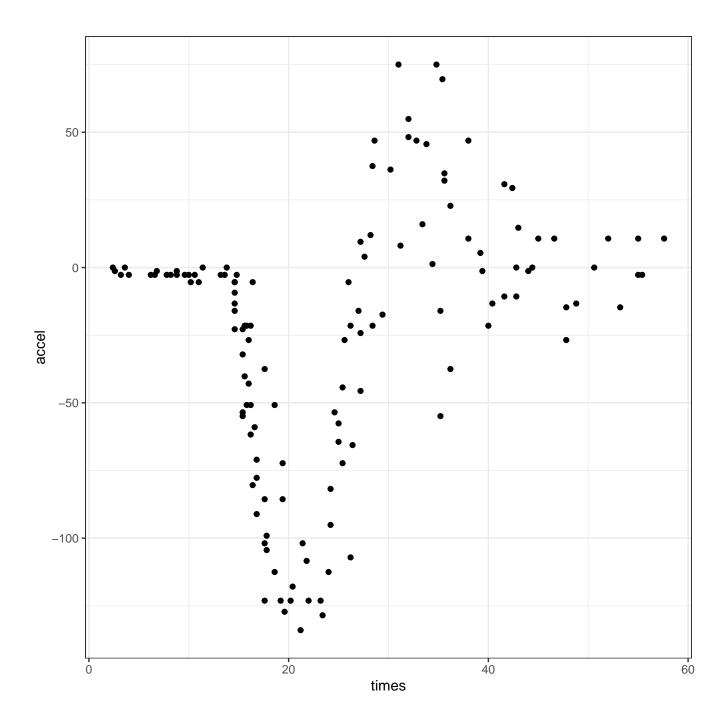


The built-in LOESS function results in a fit that does not over-fit the data, but we feel our model provides the better fit.

Problem 2

```
library(MASS)
data("mcycle")

ggplot(mcycle, aes(x = times, y = accel)) + theme_bw() + geom_point()
```



Part a

Determining LOESS regression fits on the data

Displaying data frame fit_table2

Span	Degree	RSE	
0.25	1	24.54703	
0.30	1	26.63732	
0.35	1	28.88638	
0.40	1	30.88313	
0.45	1	32.57616	
0.50	1	34.02896	
0.55	1	35.27381	
0.60	1	36.36153	
0.65	1	37.32657	
0.70	1	38.18843	
0.75	1	38.96106	
0.25	2	21.66747	
0.30	2	21.99463	
0.35	2	22.42284	
0.40	2	23.12502	
0.45	2	24.29479	
0.50	2	25.87832	
0.55	2	27.50811	
0.60	2	29.01310	
0.65	2	30.39499	
0.70	2	31.68249	
0.75	2	32.87589	
	0.25 0.30 0.35 0.40 0.45 0.50 0.65 0.70 0.75 0.25 0.30 0.45 0.50 0.55 0.60 0.65 0.70	0.30 1 0.35 1 0.40 1 0.45 1 0.50 1 0.55 1 0.60 1 0.65 1 0.70 1 0.75 1 0.25 2 0.30 2 0.35 2 0.40 2 0.45 2 0.50 2 0.55 2 0.60 2 0.65 2 0.70 2	

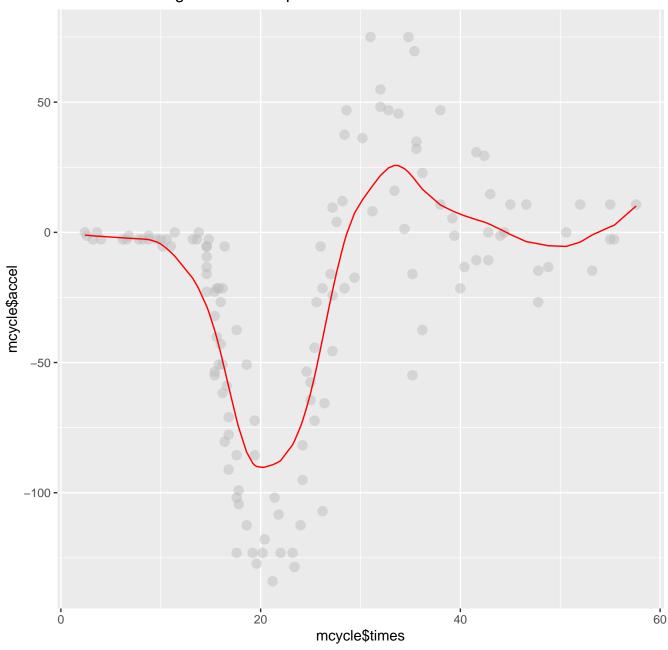
The three "best" fits with degree 1 appear to be span 0.25, 0.30, and 0.35. The three "best" fits with degree 2 appear to be span 0.25, 0.30, and 0.35.

Plotting the best fits found above

myloess(mcycle\$times, mcycle\$accel,

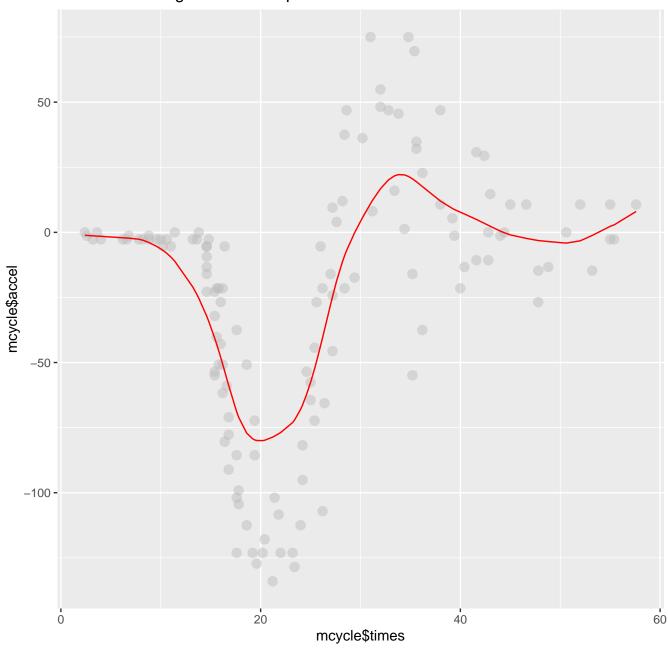
span = 0.25, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.25



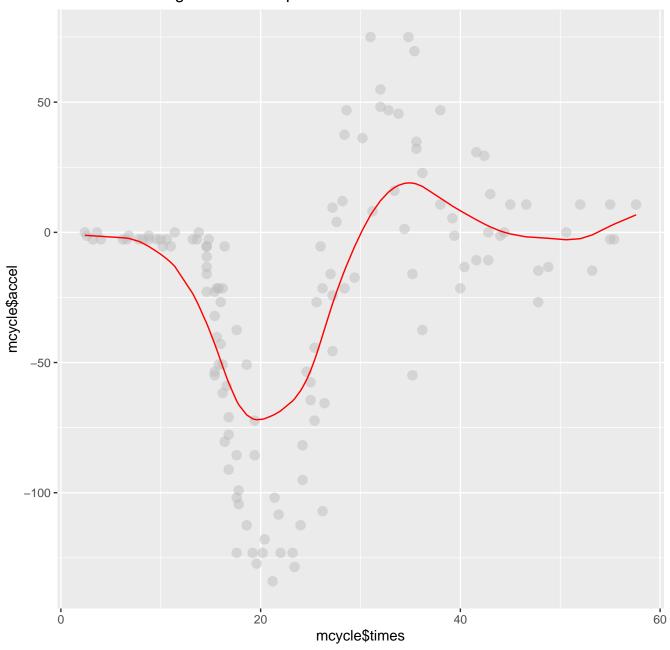
span = 0.30, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.3



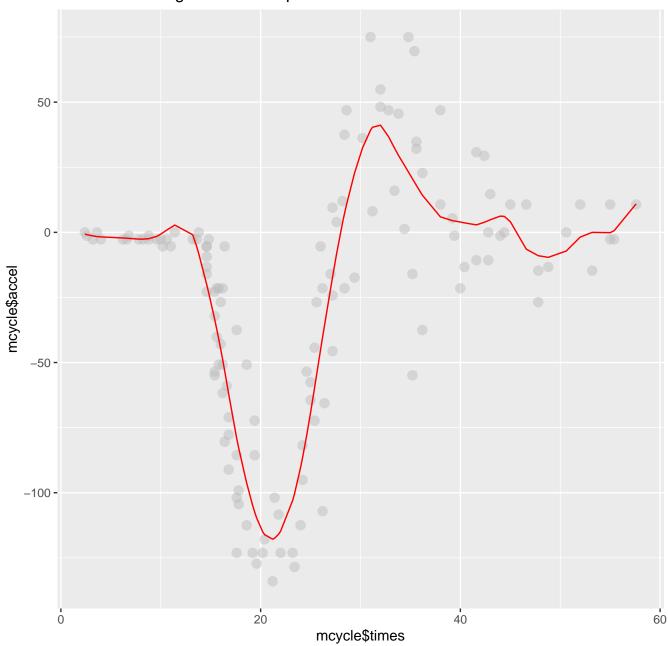
span = 0.35, degree = 1, show.plot = F)\$loessplot

LOESS with degree = 1 and span = 0.35



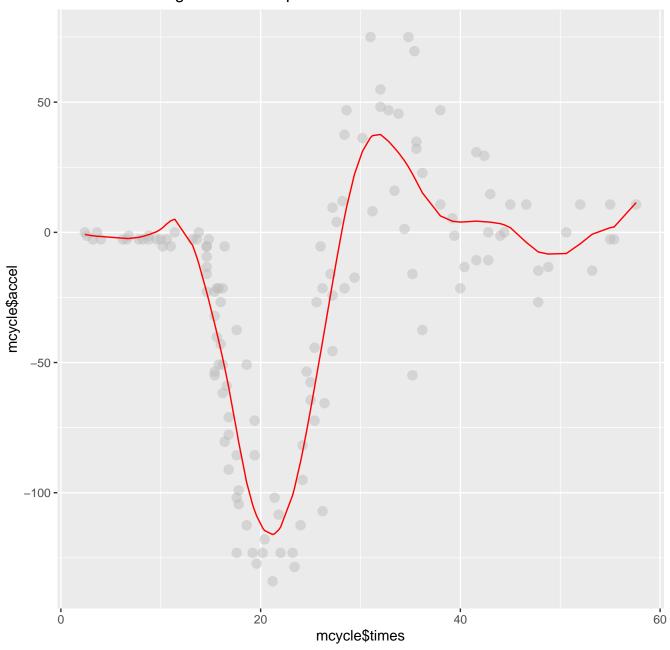
span = 0.25, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.25



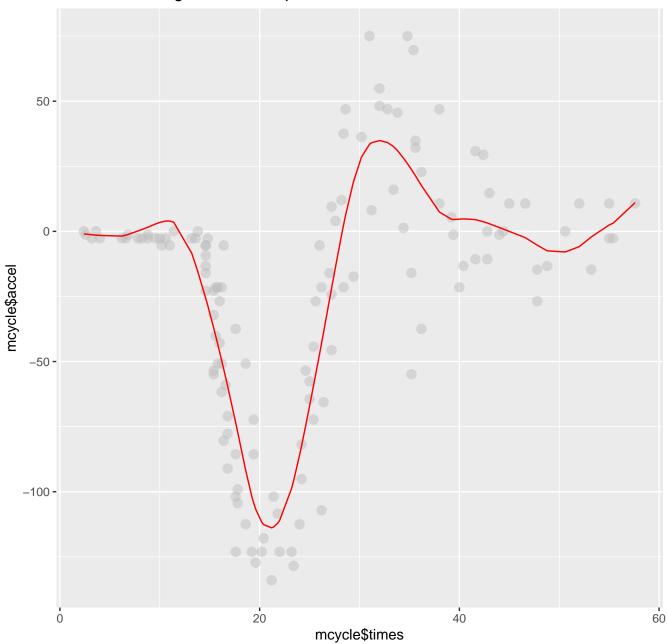
span = 0.30, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.3



span = 0.35, degree = 2, show.plot = F)\$loessplot

LOESS with degree = 2 and span = 0.35

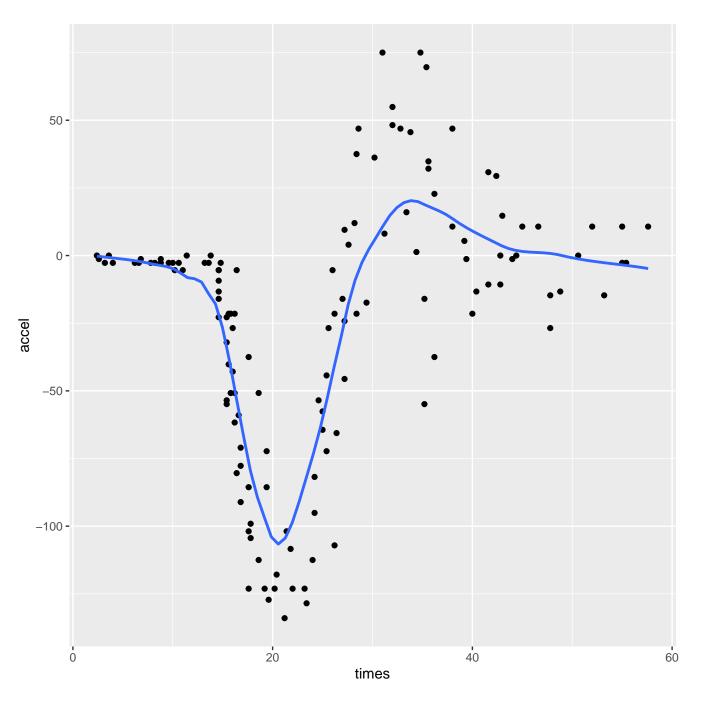


Visually inspecting the models, we believe that the model with degree 2 and span 0.35 provided the "best" fit.

Part b

Comparing results with built-in LOESS function

```
mcycle %>% ggplot(aes(times, accel)) +
  geom_point() +
  geom_smooth(method = "loess", degree = 2, span = 0.35, se = F, method.args = list(degree=1))
```



The built-in LOESS function results in a fit that does not over-fit the data, but we feel our model provides the better fit.

Problem 3

```
# Some pre-processing
library(ISLR)
# Remove the name of the car model and change the origin to categorical with actual name
Auto_new <- Auto[, -9]</pre>
# Lookup table
newOrigin <- c("USA", "European", "Japanese")</pre>
Auto_new$origin <- factor(newOrigin[Auto_new$origin], newOrigin)</pre>
# Look at the first 6 observations to see the final version
head(Auto_new)
  mpg cylinders displacement horsepower weight acceleration year origin
1 18
                          307
                                      130
                                            3504
                                                          12.0
                                                                 70
```

```
350
                               165 3693
                                                      70
                                                           USA
2 15
            8
                                                11.5
3 18
            8
                     318
                               150 3436
                                                11.0
                                                      70
                                                           USA
4 16
            8
                     304
                               150 3433
                                                12.0
                                                      70
                                                           USA
5 17
            8
                     302
                               140
                                    3449
                                                10.5
                                                      70
                                                           USA
            8
                     429
                               198 4341
                                                           USA
6 15
                                                10.0
                                                      70
```

Writing the function that carries out kNN classification and regression

```
library(caret)
```

```
# This function has the following inputs
# * train - matrix or data frame of training set cases
# * test - matrix or data frame of test set cases.
      (A vector will be interpreted as a row vector for a single case.)
# * y_train - Either a numeric vector, or factor vector for the responses in the training set
# * y_test - Either a numeric vector, or factor vector for the responses in the testing set
# * k - number of neighbors considered, the default value is 3
# If weighted = TRUE, then function uses the distance weighted kNN,
# otherwise it does the default kNN method.
mykNN <- function(train, test, y_train, y_test, k = 3, weighted = TRUE) {
  # Allocating space for vector of fitted values
  yhat <- vector(mode = "numeric", length = length(y_test))</pre>
  # Fitting each point
  for (row in 1:nrow(test)) {
    # Getting features
    x0 <- test[row,]</pre>
    # Getting Euclidean distance and weights
    distmat <- as.matrix(dist(rbind(x0, train), method = "euclidean", diag = T, upper = T))</pre>
    dist <- distmat[1,]</pre>
    weights <- 1/dist
    # Getting kth nearest neighbor
    a.order <- order(weights, decreasing = T)[-1]</pre>
    last <- weights[a.order[k]]</pre>
    # Setting weights to 0 except for kNN
    y_train_sub <- y_train[-which(!is.finite(weights))]</pre>
    weights <- weights[-which(!is.finite(weights))]</pre>
    weights[weights < last] <- 0</pre>
    # Handling unweighted case
    if(weighted == F) {
      weights[weights != 0] <- 1
    tot_weight <- sum(weights)</pre>
    # Handling classification
    if (is.factor(y_train)) {
      # Allocating space for vector of class weights
      class <- vector(mode = "numeric", length = nlevels(y_test))</pre>
      # Summing weights for each class
```

```
for (i in 1:nlevels(y_test)) {
      class[i] <- sum(weights[which(y_train == levels(y_test)[i])])</pre>
    # Assigning factor with highest class weight to yhat
    yhat[row] <- levels(y_test)[which(class == max(class))]</pre>
  }
  # Handling regression
  else {
    # Calculating yhat
    yhat[row] <- sum(weights*y_train/tot_weight)</pre>
  }
}
# Handling classification
if (is.factor(y_train)) {
  yhat <- factor(yhat)</pre>
  # Setting number of correct predictions to 0
  num correct <- 0
  # Getting number of correct predictions
  for (j in 1:length(yhat)) {
    # Checking if classes match
    if (y_test[j] == yhat[j]) {
      num_correct <- num_correct + 1</pre>
    }
  }
  # Calculating accuracy and error rate
  accuracy <- num_correct / length(yhat)</pre>
  error_rate <- 1 - accuracy
  # Getting confusion matrix
  confmat <- confusionMatrix(yhat, y_test)</pre>
  # Returning named list
  return(invisible(list(yhat = yhat, accuracy = accuracy,
                         error_rate = error_rate, confmat = confmat, k = k)))
}
# Handling regression
else {
  # Calculating residuals, SSE, MSE, and residual standard error
  residuals <- y_test - yhat
  SSE <- sum(residuals^{2})</pre>
 MSE <- SSE/(nrow(test)-2)</pre>
 RSE <- sqrt(MSE)
  # Returning named list
  return(invisible(list(yhat = yhat, residuals = residuals, SSE = SSE, k = k)))
}
```

}

```
Splitting data into training data and testing data
ntrain <- round(nrow(Auto_new)*0.7)</pre>
ntest <- nrow(Auto new) - ntrain</pre>
train <- Auto_new[1:ntrain,1:7]</pre>
test <- Auto_new[(ntrain+1):nrow(Auto_new),1:7]</pre>
y_train <- Auto_new[1:ntrain,8]</pre>
y_test <- Auto_new[(ntrain+1):nrow(Auto_new),8]</pre>
Determining accuracy of kNN function on the data
# Creating an empty data frame
acc_table <- data.frame()</pre>
# Determining fits and putting info into data frame
for (i in c(1, 3, 5, 10, 20)) {
  acc_table <- rbind(acc_table, c("False", i, mykNN(train, test, y_train, y_test, k = i, weighted = F)$accurac
  acc_table <- rbind(acc_table, c("True", i, mykNN(train, test, y_train, y_test, k = i)$accuracy))</pre>
}
# Changing column names
colnames(acc_table) <- c("Weighted", "k", "Accuracy")</pre>
# Displaying data frame
acc_table
   Weighted k
                         Accuracy
      False 1 0.559322033898305
1
2
      True 1 0.559322033898305
3
      False 3 0.542372881355932
4
      True 3 0.576271186440678
5
    False 5 0.559322033898305
6
      True 5 0.550847457627119
7
     False 10 0.593220338983051
8
      True 10 0.567796610169492
      False 20 0.550847457627119
9
10
       True 20 0.584745762711864
# Displaying confusion matrix of best fit
best <- mykNN(train, test, y_train, y_test, k = 9, weighted = F)</pre>
best$confmat
Confusion Matrix and Statistics
          Reference
Prediction USA European Japanese
            47
                    11
  European
            9
                      5
                                8
  Japanese
             5
                               20
Overall Statistics
               Accuracy : 0.6102
                  95% CI: (0.5161, 0.6986)
    No Information Rate: 0.5169
    P-Value [Acc > NIR] : 0.02613
                   Kappa: 0.3479
 Mcnemar's Test P-Value: 0.44429
```

Statistics by Class:

	Class: USA	Class: European	Class: Japanese
Sensitivity	0.7705	0.25000	0.5405
Specificity	0.6491	0.82653	0.8889
Pos Pred Value	0.7015	0.22727	0.6897
Neg Pred Value	0.7255	0.84375	0.8090
Prevalence	0.5169	0.16949	0.3136
Detection Rate	0.3983	0.04237	0.1695
Detection Prevalence	0.5678	0.18644	0.2458
Balanced Accuracy	0.7098	0.53827	0.7147

Problem 4

Part a

```
ntrain <- round(nrow(ozone)*0.63)</pre>
ntest <- nrow(ozone) - ntrain</pre>
train <- ozone[1:ntrain,3]</pre>
test <- ozone[(ntrain+1):nrow(ozone),3]</pre>
y_train <- ozone[1:ntrain,1]</pre>
y_test <- ozone[(ntrain+1):nrow(ozone),1]</pre>
'# Creating an empty data frame
acc_table2 <- data.frame()</pre>
# Determining fits and putting info into data frame
for (i in c(1, 3, 5, 10, 20)) {
  acc_table2 <- rbind(acc_table2, c("False", i, mykNN(train, test, y_train, y_test, k = i, weighted = F)$SSE))</pre>
  acc_table2 <- rbind(acc_table2, c("True", i, mykNN(train, test, y_train, y_test, k = i)$SSE))</pre>
# Changing column names
colnames(acc_table2) <- c("Weighted", "k", "SSE")</pre>
# Displaying data frame
acc_table2'
[1] "# Creating an empty data frame\nacc_table2 <- data.frame()\n\n# Determining fits and putting info into da
```

Part b

```
'best <- mykNN(train, test, y_train, y_test, k = 1)'
[1] "best <- mykNN(train, test, y_train, y_test, k = 1)"</pre>
```