CMDA-4654

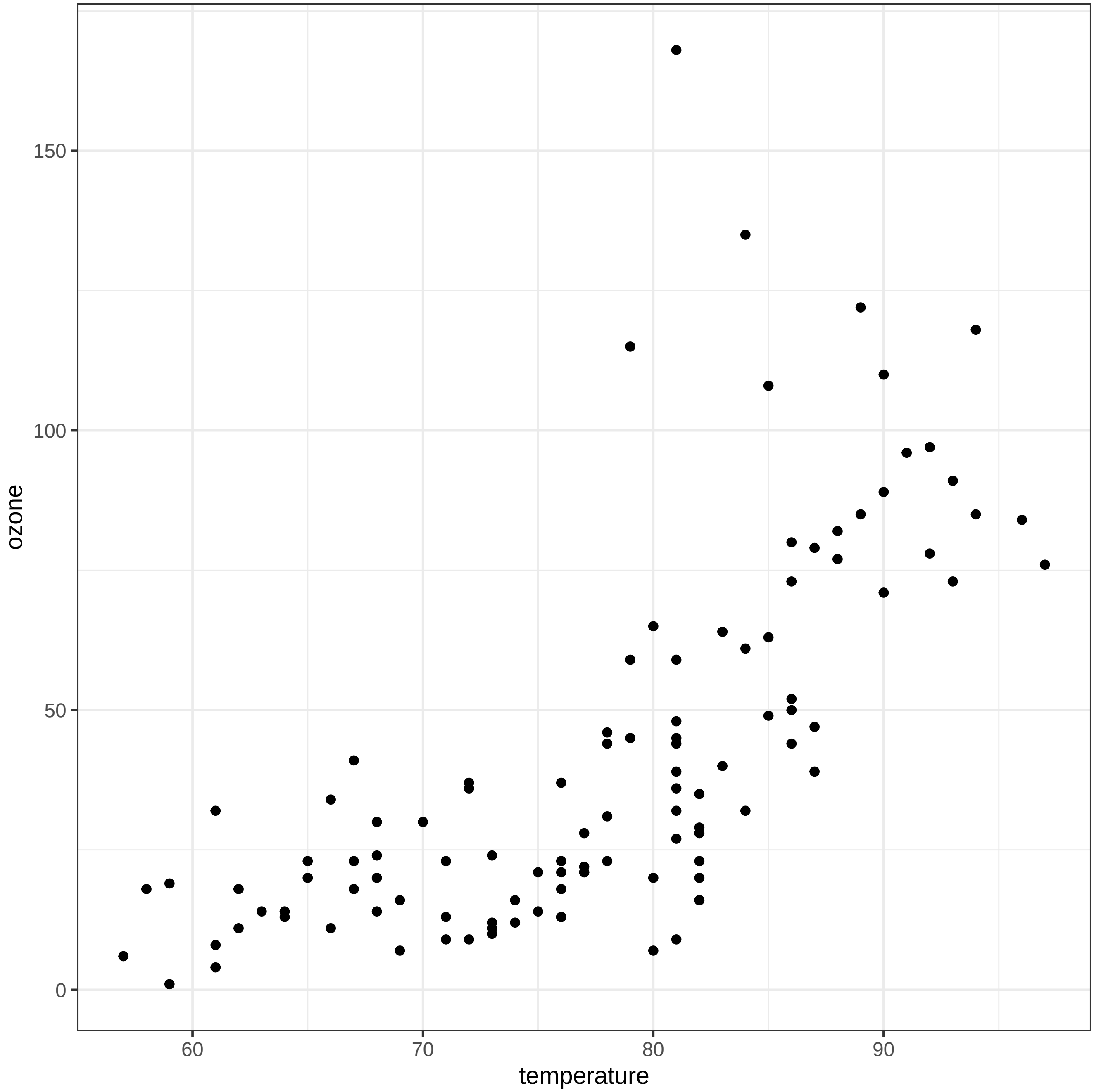
Project 1

Spencer Paragas and Christopher Mascis

10/19/2021

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)
```

```r
model5 <- lm(ozone ~ poly(radiation,5), data = ozone)
model6 <- lm(ozone ~ poly(radiation,6), data = ozone)

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
```

```r
summary(model2)
```

```
Call:
lm(formula = ozone ~ poly(radiation, 2), data = ozone)

Residuals:
    Min      1Q  Median      3Q     Max 
-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
```

```r
summary(model3)
```

```
Call:
lm(formula = ozone ~ poly(radiation, 3), data = ozone)

Residuals:
   Min     1Q Median     3Q    Max 
-45.05 -19.44  -4.52  15.61 109.95 

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)    
(Intercept)            42.10       2.78  15.141  < 2e-16 ***
poly(radiation, 3)1   121.57      29.29   4.150 6.69e-05 ***
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 '**' 0.01 '*' 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
```

```r
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|)
(Intercept)           42.099      2.793  15.072  < 2e-16 ***
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 '**' 0.01 '*' 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
```

```r
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 *
poly(radiation, 5)4    4.777     29.511   0.162 0.871718
poly(radiation, 5)5   18.759     29.511   0.636 0.526389
---
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
```

```r
summary(model6)
```

```
Call:
lm(formula = ozone ~ poly(radiation, 6), data = ozone)

Residuals:
```

```
    Min      1Q  Median      3Q     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 *  
poly(radiation, 6)4    4.777     29.626   0.161  0.87221    
poly(radiation, 6)5   18.759     29.626   0.633  0.52800    
poly(radiation, 6)6  -12.854     29.626  -0.434  0.66527    
---
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

```
myloess <- function(x, y, span = 0.5, degree = 1, show.plot = TRUE) {

  # Getting range of values
  xrange <- diff(range(x))

  # Checking span meets requirements and setting width
  if (between(span, 0, 1)) {
    width <- span*xrange
  }
  else {
    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)
  Win_total <- length(x)

  # Allocating space for vector of each window's population
  n_points <- vector(mode = "integer", length = length(x))

  # Allocating space for vector of fitted values
  yhat <- vector(mode = "numeric", length = length(x))

  # Combining our variables in data frame
  mydata <- cbind.data.frame(x, y)

  # Fitting each point
  for(x0 in x) {

    # Setting population of window
    sample <- subset(mydata, between(x, x0-width/2, x0+width/2))
    n <- length(sample[,1])

    # Getting weights into diagonal matrix
    weights <- (1-(abs(sample[,1] - x0)/width*2)^3)^3
    W_mat <- diag(weights, n, n)
```

```
    # Checking degree and completing our regression accordingly
    if (degree == 1) {

      X_mat <- cbind(rep(1, n), sample[,1])
      betahat <- solve( t(X_mat)%*%W_mat%*%X_mat ) %*% t(X_mat) %*% W_mat %*% sample[,2]

      # Getting fitted value
      yhat[which(x0 == x)] <-  betahat[1] + betahat[2]*x0
    }
    else if (degree == 2) {

      X_mat <- cbind(rep(1, n), sample[,1], sample[,1]^2)
      betahat <- solve( t(X_mat)%*%W_mat%*%X_mat ) %*% t(X_mat) %*% W_mat %*% sample[,2]

      # Getting fitted value
      yhat[which(x0 == x)] <-  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})
  MSE <- SSE/(N_total-2)
  RSE <- sqrt(MSE)

  # Creating plot of final fit
  loessplot <- ggplot(mydata, aes(x, y)) +
    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()

# 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,
                                                  span = i, degree = j, show.plot = F)$RSE))
  }
}
```

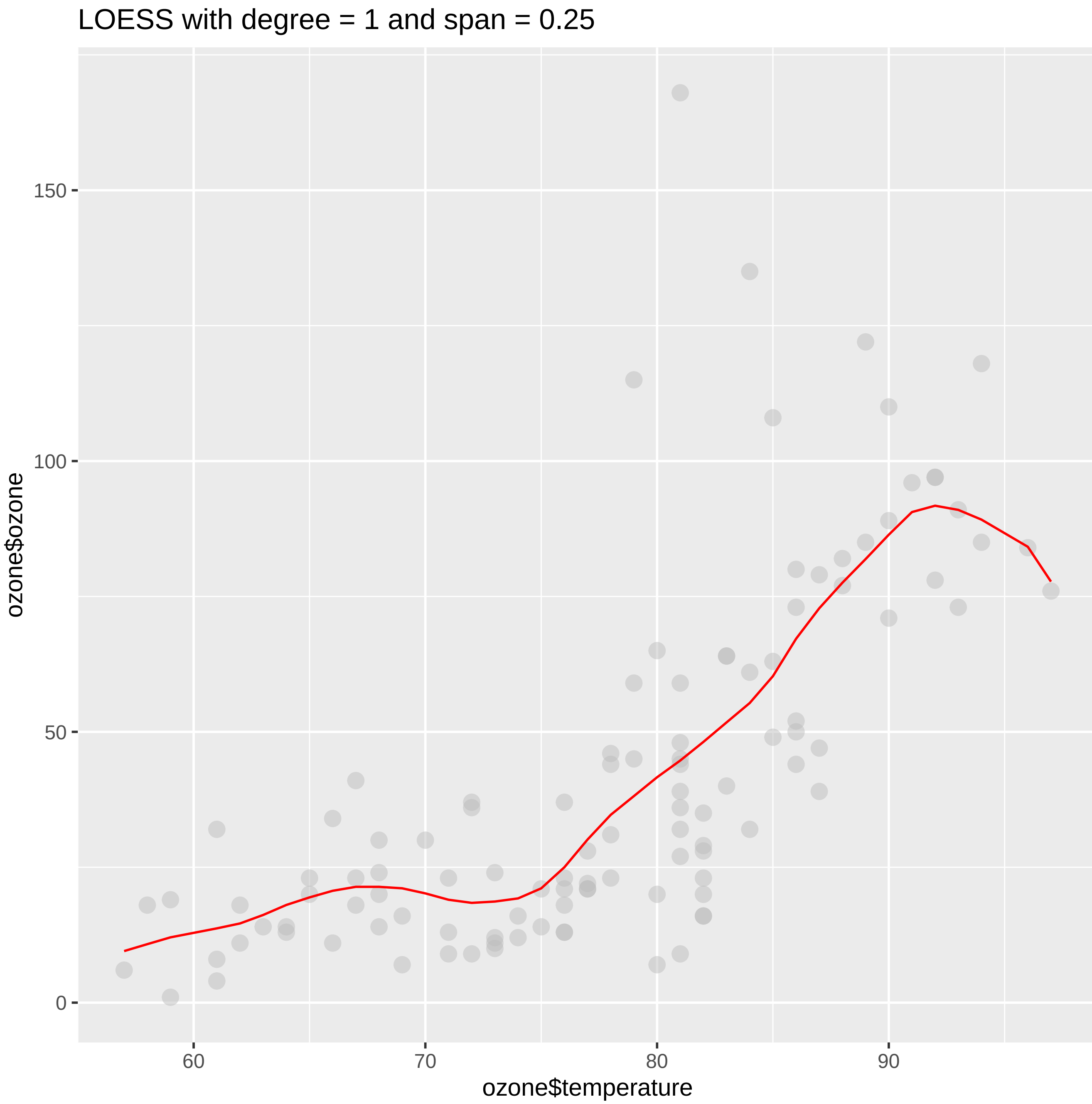
```r
# Changing column names
colnames(fit_table) <- c("Span", "Degree", "RSE")

# 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
6  0.50      1 21.92533
7  0.55      1 21.98316
8  0.60      1 22.05339
9  0.65      1 22.12531
10 0.70      1 22.18786
11 0.75      1 22.24218
12 0.25      2 20.70123
13 0.30      2 21.21788
14 0.35      2 21.65352
15 0.40      2 21.83486
16 0.45      2 21.82088
17 0.50      2 21.75230
18 0.55      2 21.71153
19 0.60      2 21.71786
20 0.65      2 21.76031
21 0.70      2 21.81288
22 0.75      2 21.86516
```

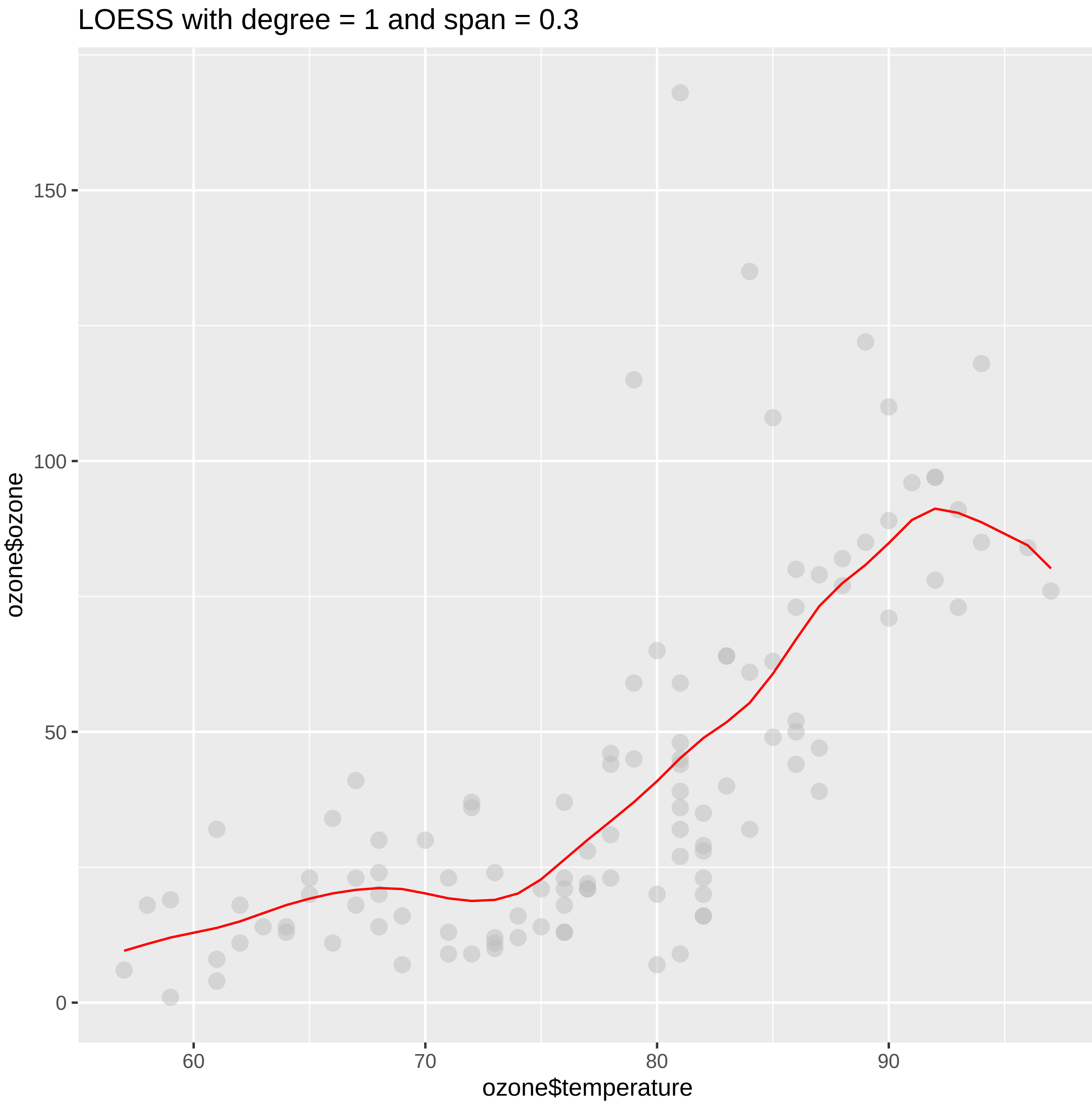
The three "best" fits with degree 1 appear to be span 0.25, 0.30, and 0.40. The three "best" fits with degree 2 appear to be span 0.25, 0.30, and 0.35.

Plotting the best fits found above

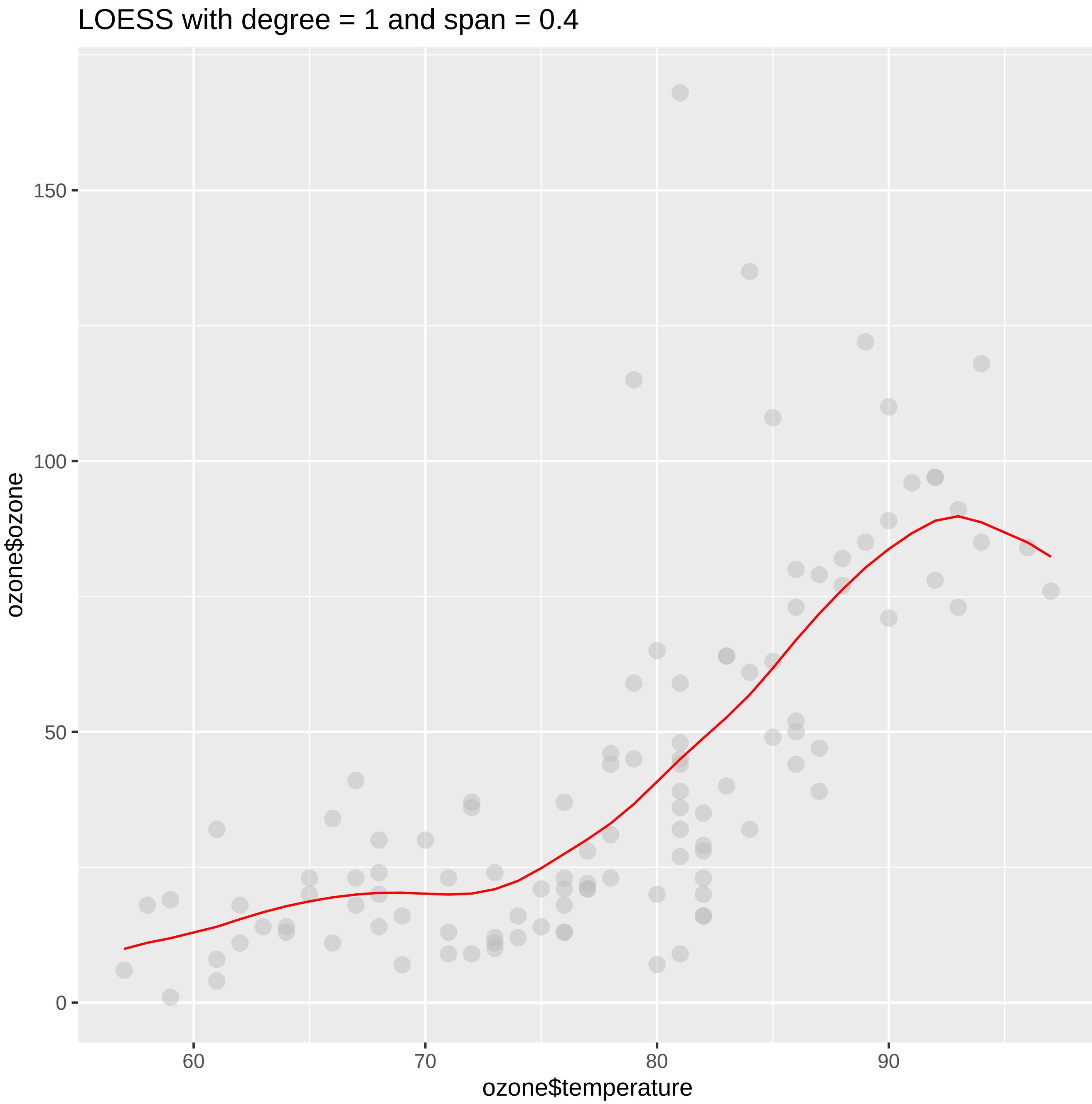
```r
myloess(ozone$temperature, ozone$ozone,
                                                  span = 0.25, degree = 1, show.plot = F)$loessplot
```



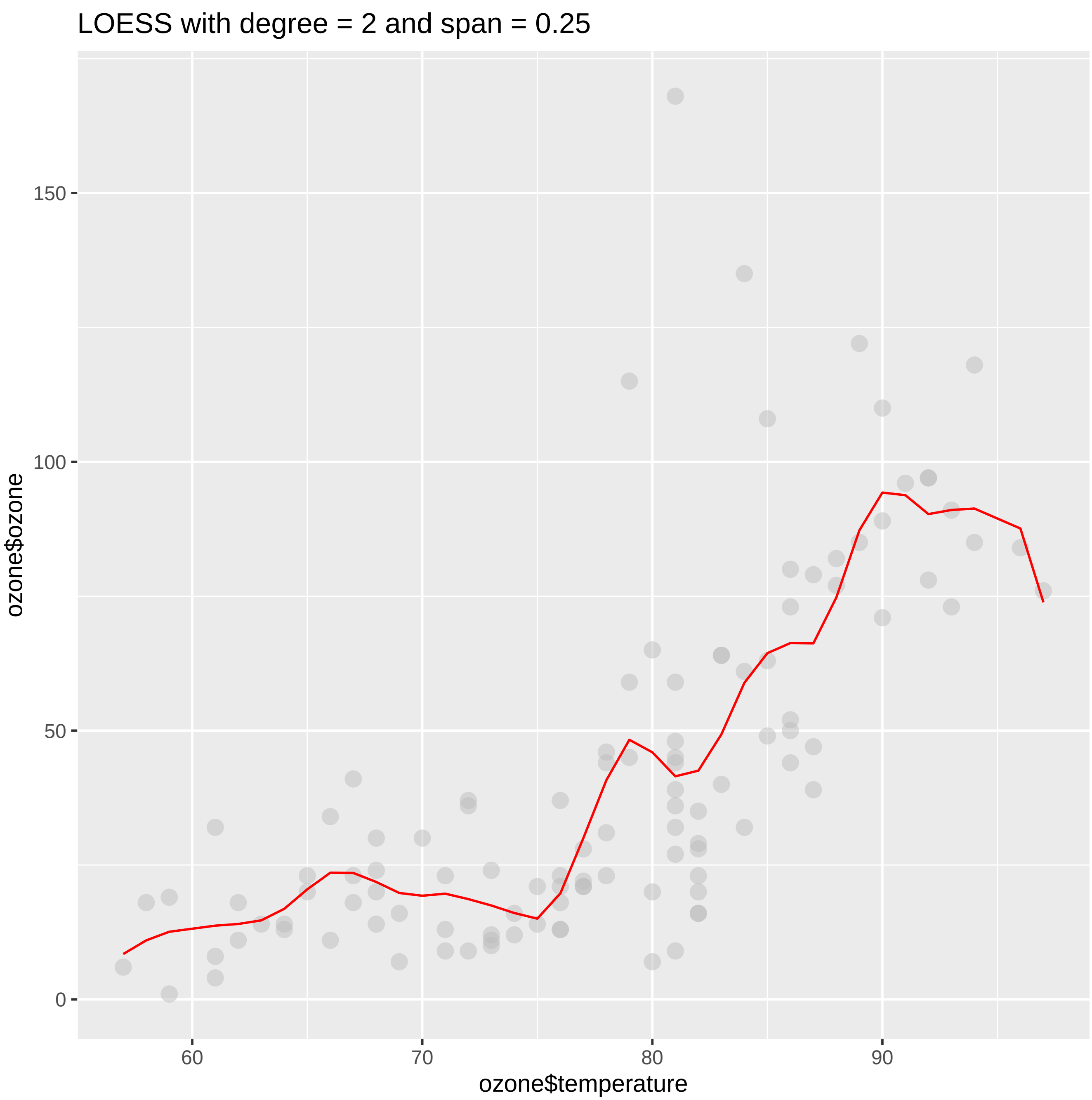

```
myloess(ozone$temperature, ozone$ozone,
                                    span = 0.30, degree = 1, show.plot = F)$loessplot
```



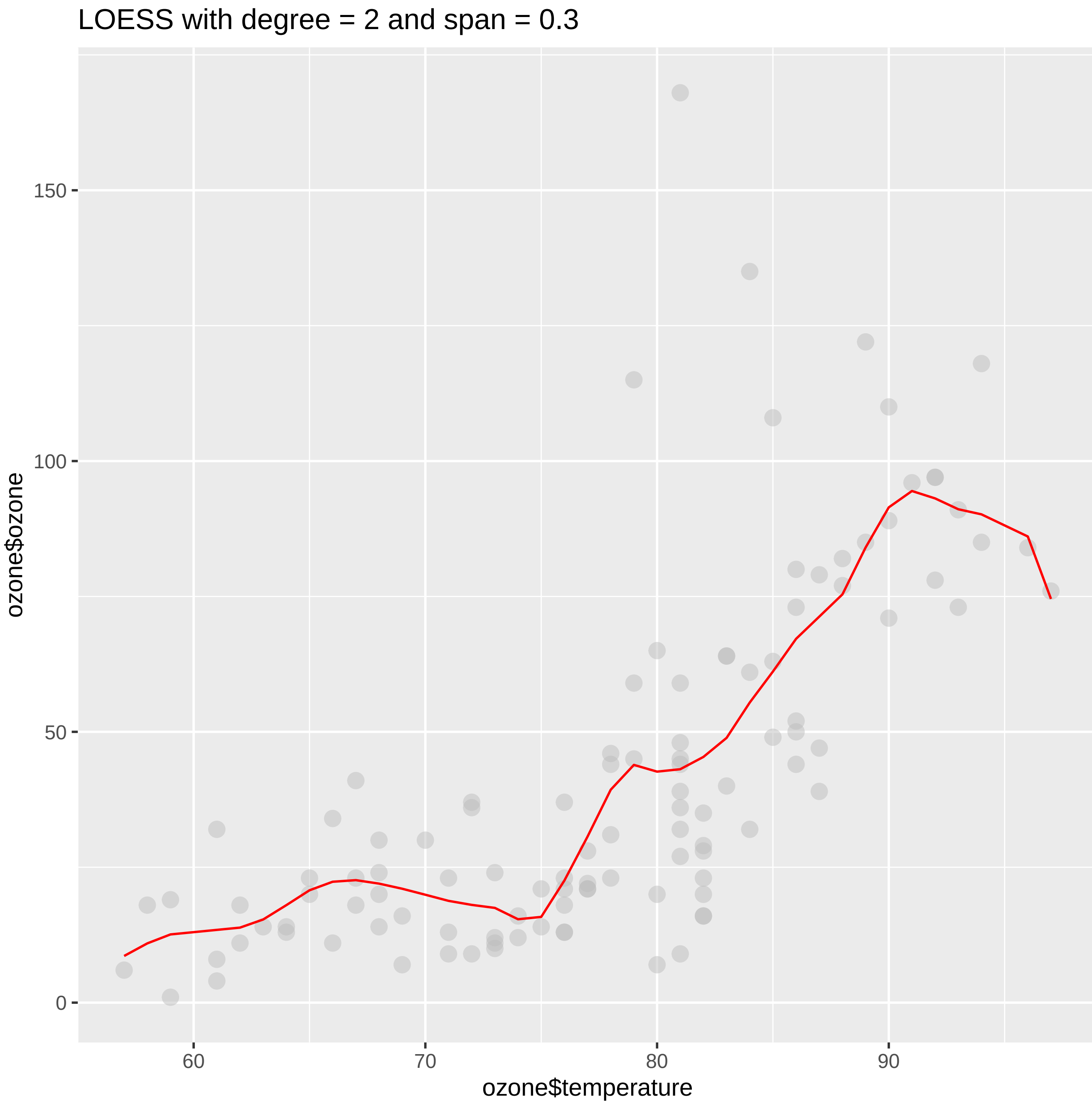

```
myloess(ozone$temperature, ozone$ozone,
                                                    span = 0.40, degree = 1, show.plot = F)$loessplot
```



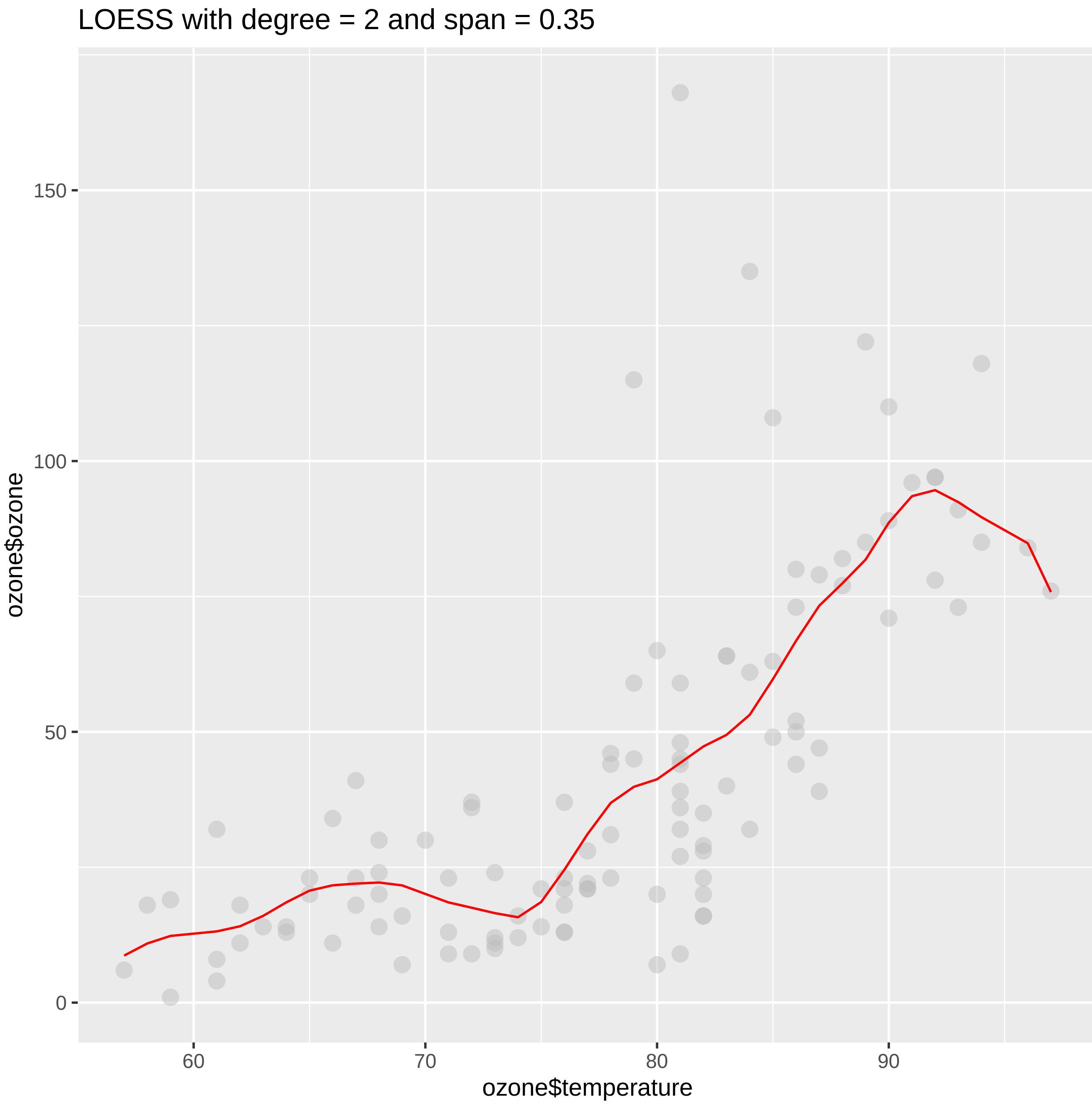

```
myloess(ozone$temperature, ozone$ozone,
                                           span = 0.25, degree = 2, show.plot = F)$loessplot
```




```
myloess(ozone$temperature, ozone$ozone,
                                                    span = 0.30, degree = 2, show.plot = F)$loessplot
```




```
myloess(ozone$temperature, ozone$ozone,
                                                span = 0.35, degree = 2, show.plot = F)$loessplot
```

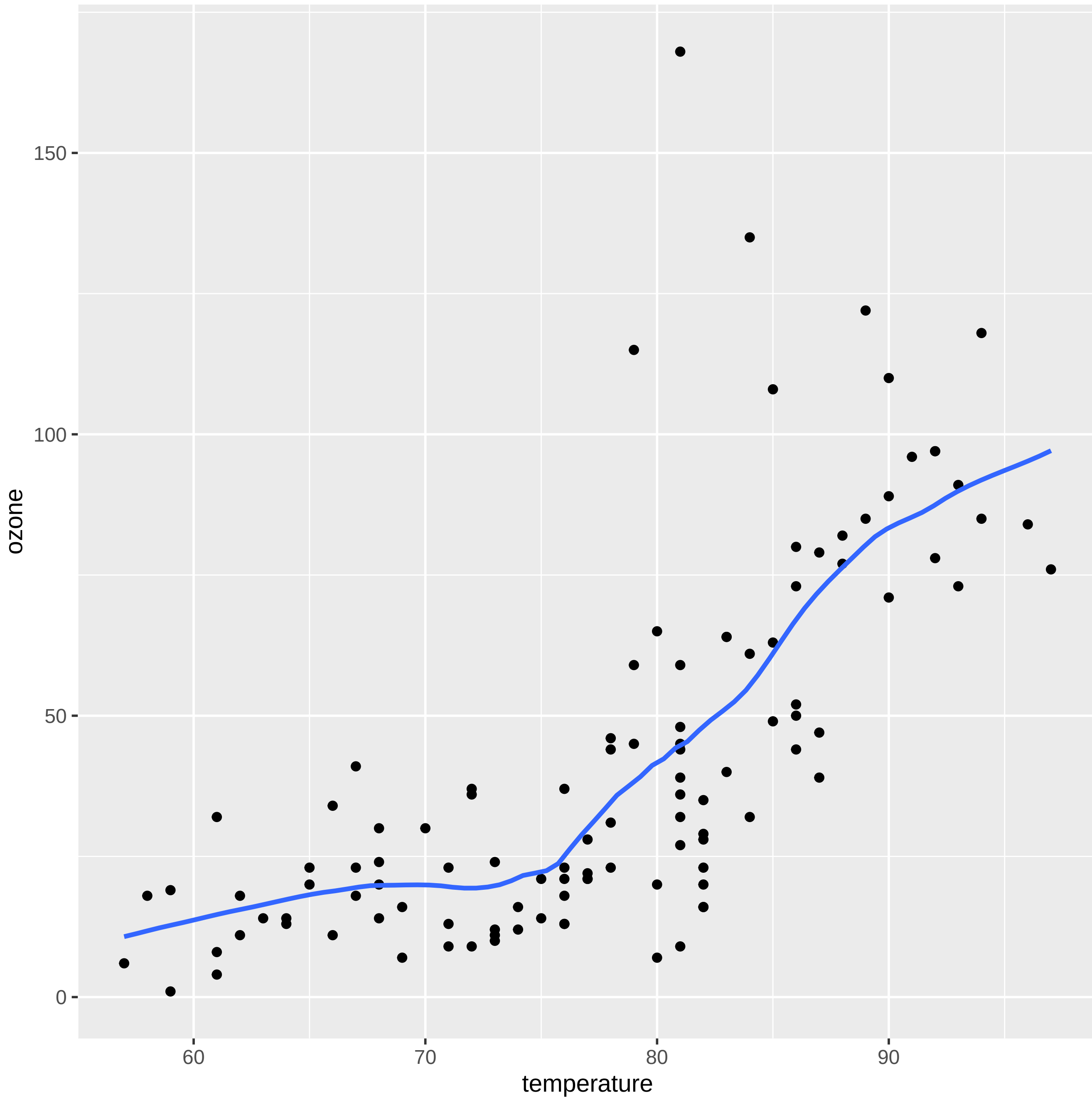


Visually inspecting the best fits compared to the 2nd and 3rd best fits, we do feel we may have over-fit the data, especially for the fits with degree 2. The model with degree 1 and span 0.4 appears to be the "best" fit.

Part c

Comparing results with built-in LOESS function

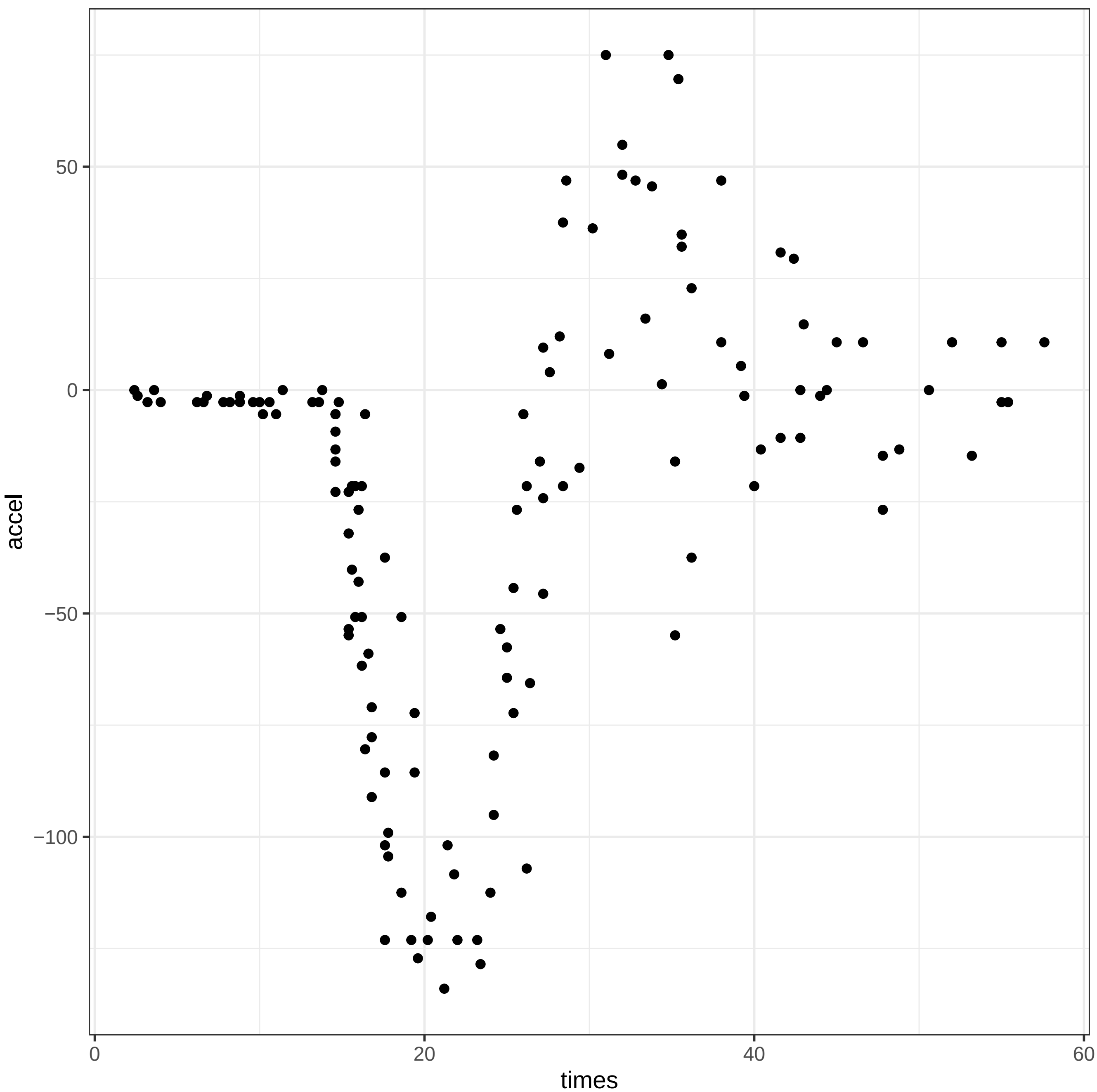
```
ozone %>% ggplot(aes(temperature, ozone)) +
  geom_point() +
  geom_smooth(method = "loess", degree = 1, span = 0.40, se = F, method.args = list(degree=1))
```



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

```
# Creating an empty data frame
fit_table2 <- data.frame()

# 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_table2 <- rbind(fit_table2, c(i, j, myloess(mcycle$times, mcycle$accel,
                                                  span = i, degree = j, show.plot = F)$RSE))
  }
}

# Changing column names
colnames(fit_table2) <- c("Span", "Degree", "RSE")
```

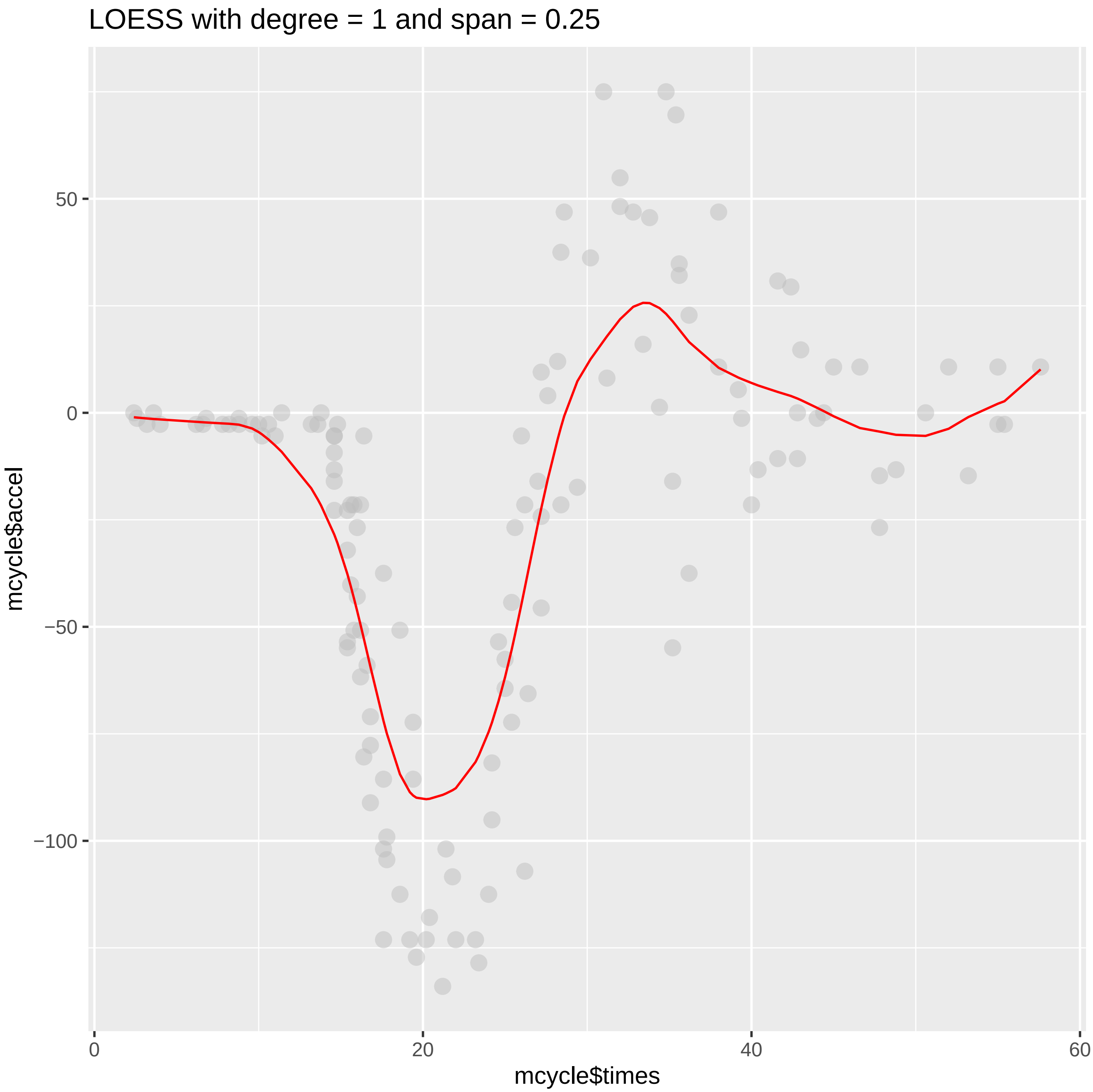
```r
# Displaying data frame
fit_table2
```

```
   Span Degree      RSE
1  0.25      1 24.54703
2  0.30      1 26.63732
3  0.35      1 28.88638
4  0.40      1 30.88313
5  0.45      1 32.57616
6  0.50      1 34.02896
7  0.55      1 35.27381
8  0.60      1 36.36153
9  0.65      1 37.32657
10 0.70      1 38.18843
11 0.75      1 38.96106
12 0.25      2 21.66747
13 0.30      2 21.99463
14 0.35      2 22.42284
15 0.40      2 23.12502
16 0.45      2 24.29479
17 0.50      2 25.87832
18 0.55      2 27.50811
19 0.60      2 29.01310
20 0.65      2 30.39499
21 0.70      2 31.68249
22 0.75      2 32.87589
```

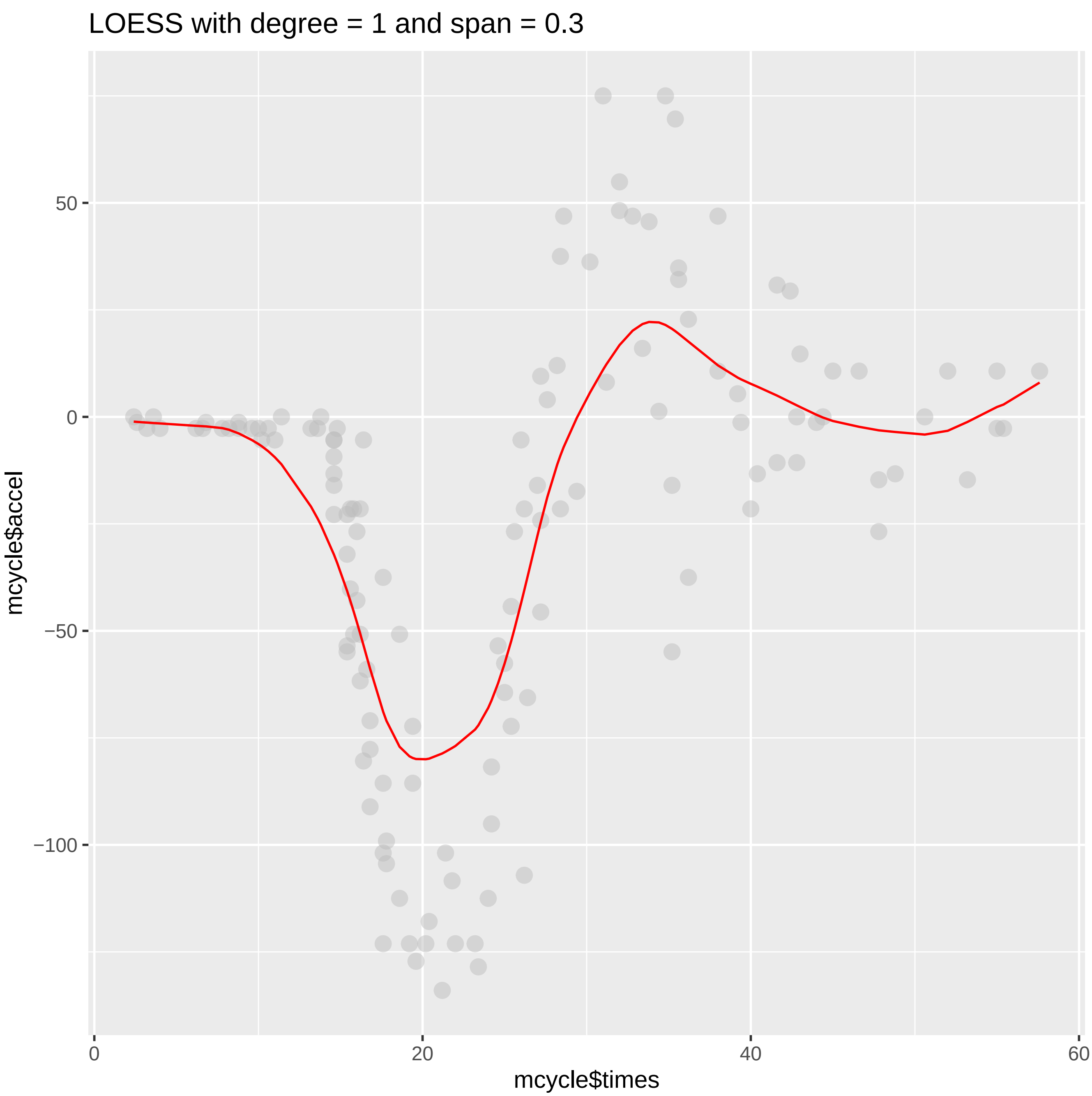
The three "best" fits with degree 1 appear to be span 0.25, 0.30, and 0.35. The three "best" fits with degree 2 appear to be span 0.25, 0.30, and 0.35.

Plotting the best fits found above

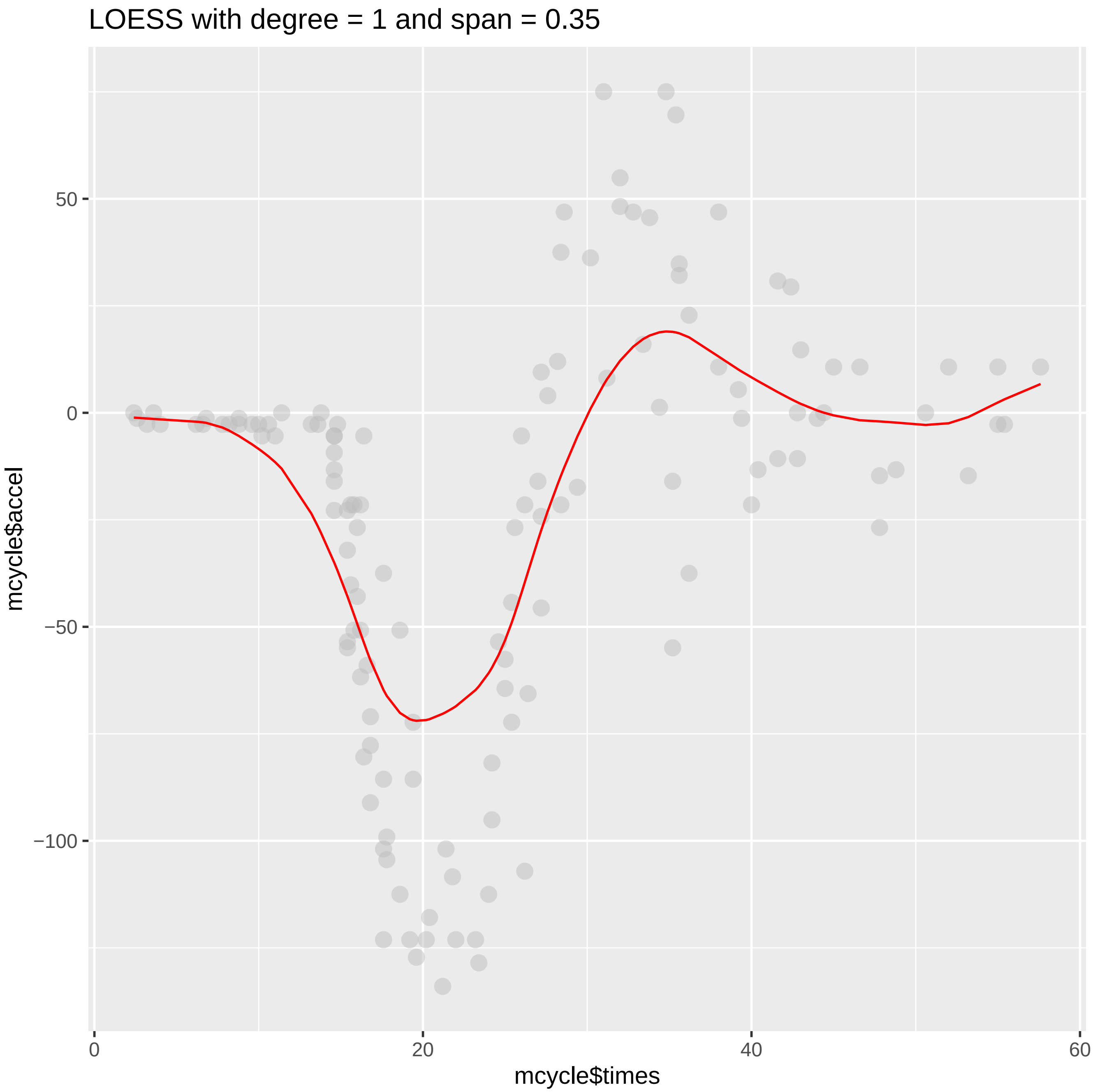
```r
myloess(mcycle$times, mcycle$accel,
                                                  span = 0.25, degree = 1, show.plot = F)$loessplot
```



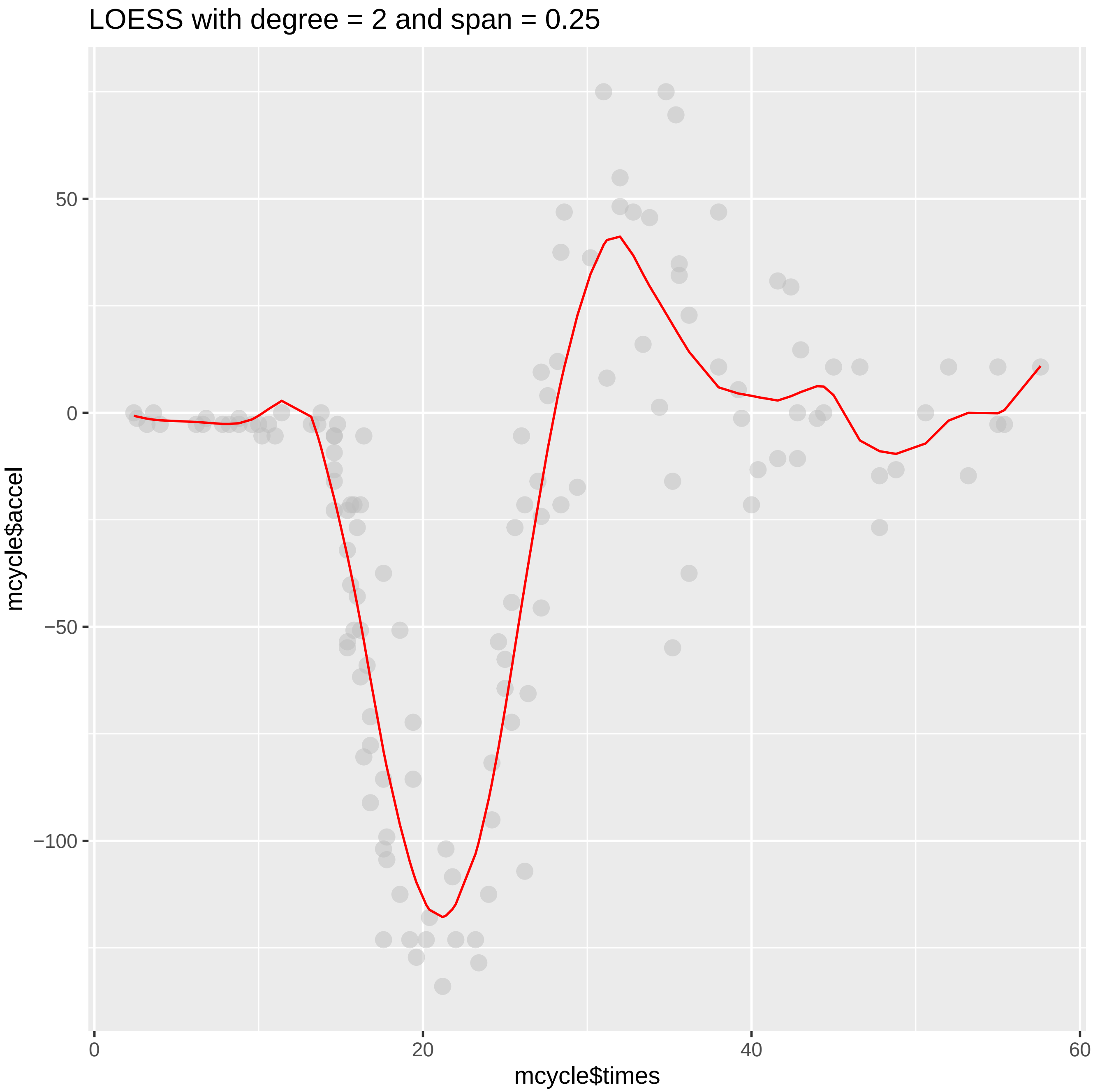

```
myloess(mcycle$times, mcycle$accel,
                                        span = 0.30, degree = 1, show.plot = F)$loessplot
```



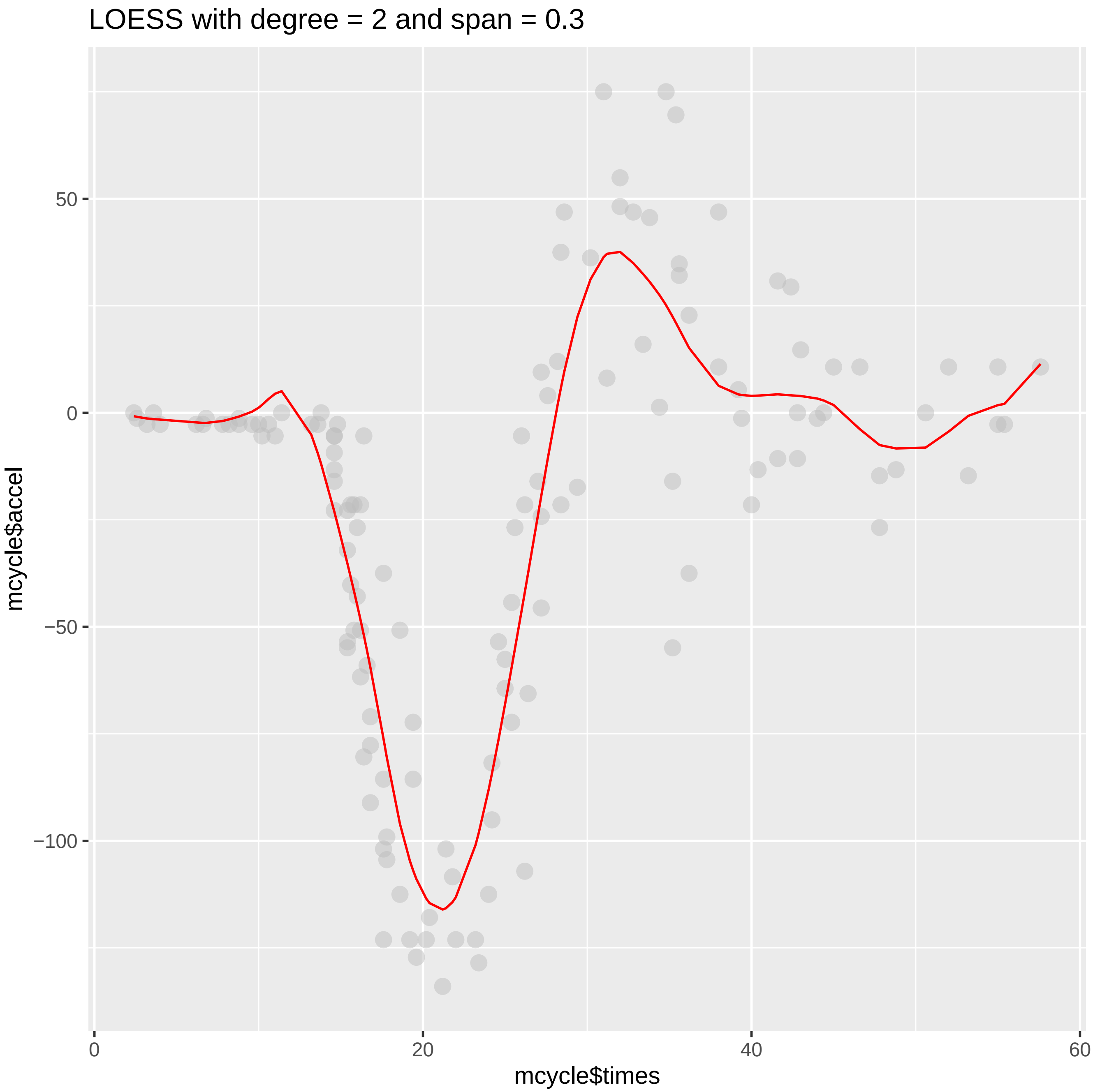

```
myloess(mcycle$times, mcycle$accel,
                                        span = 0.35, degree = 1, show.plot = F)$loessplot
```



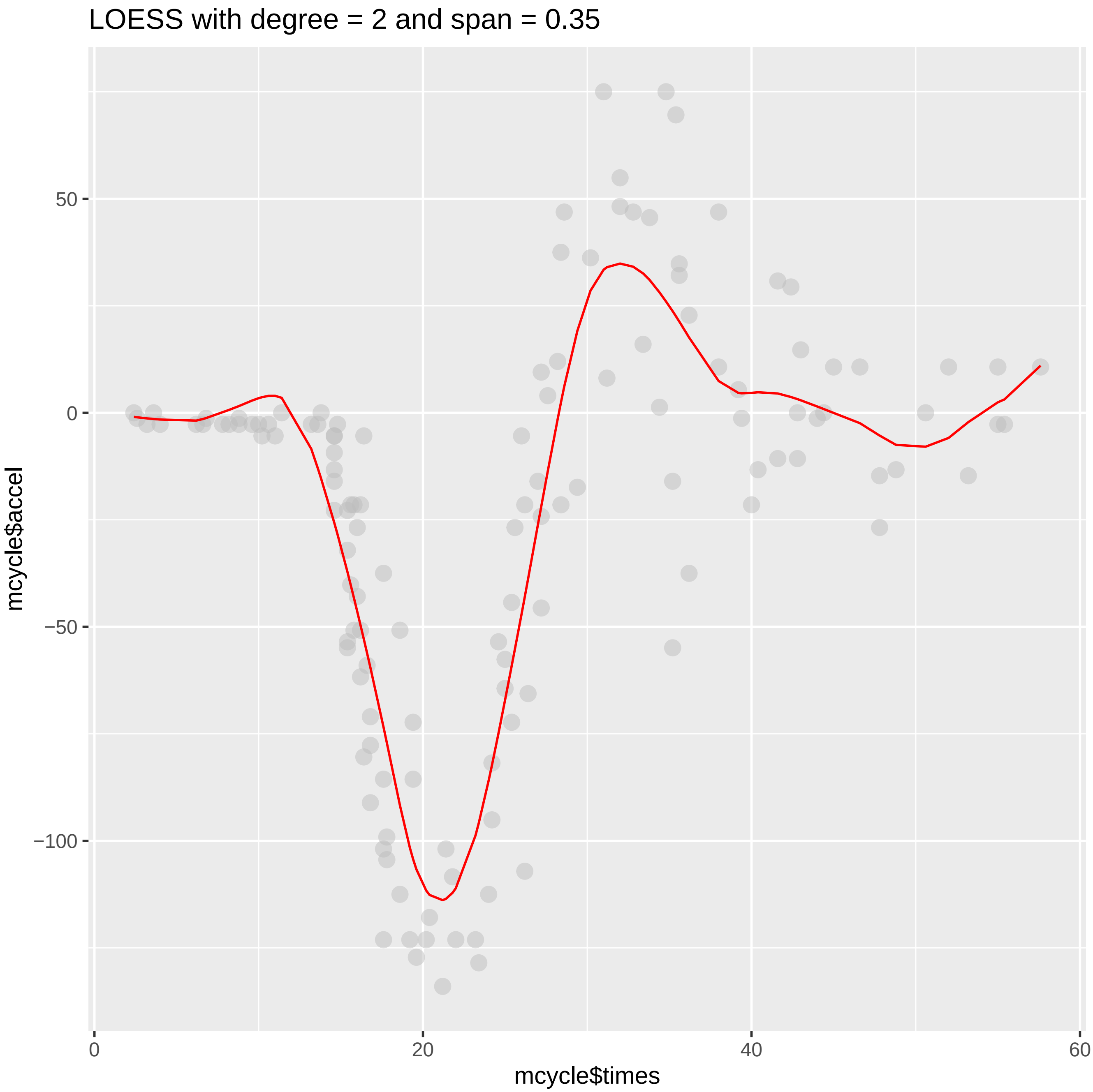

```
myloess(mcycle$times, mcycle$accel,
                                        span = 0.25, degree = 2, show.plot = F)$loessplot
```




```
myloess(mcycle$times, mcycle$accel,
                                              span = 0.30, degree = 2, show.plot = F)$loessplot
```




```
myloess(mcycle$times, mcycle$accel,
                    span = 0.35, degree = 2, show.plot = F)$loessplot
```

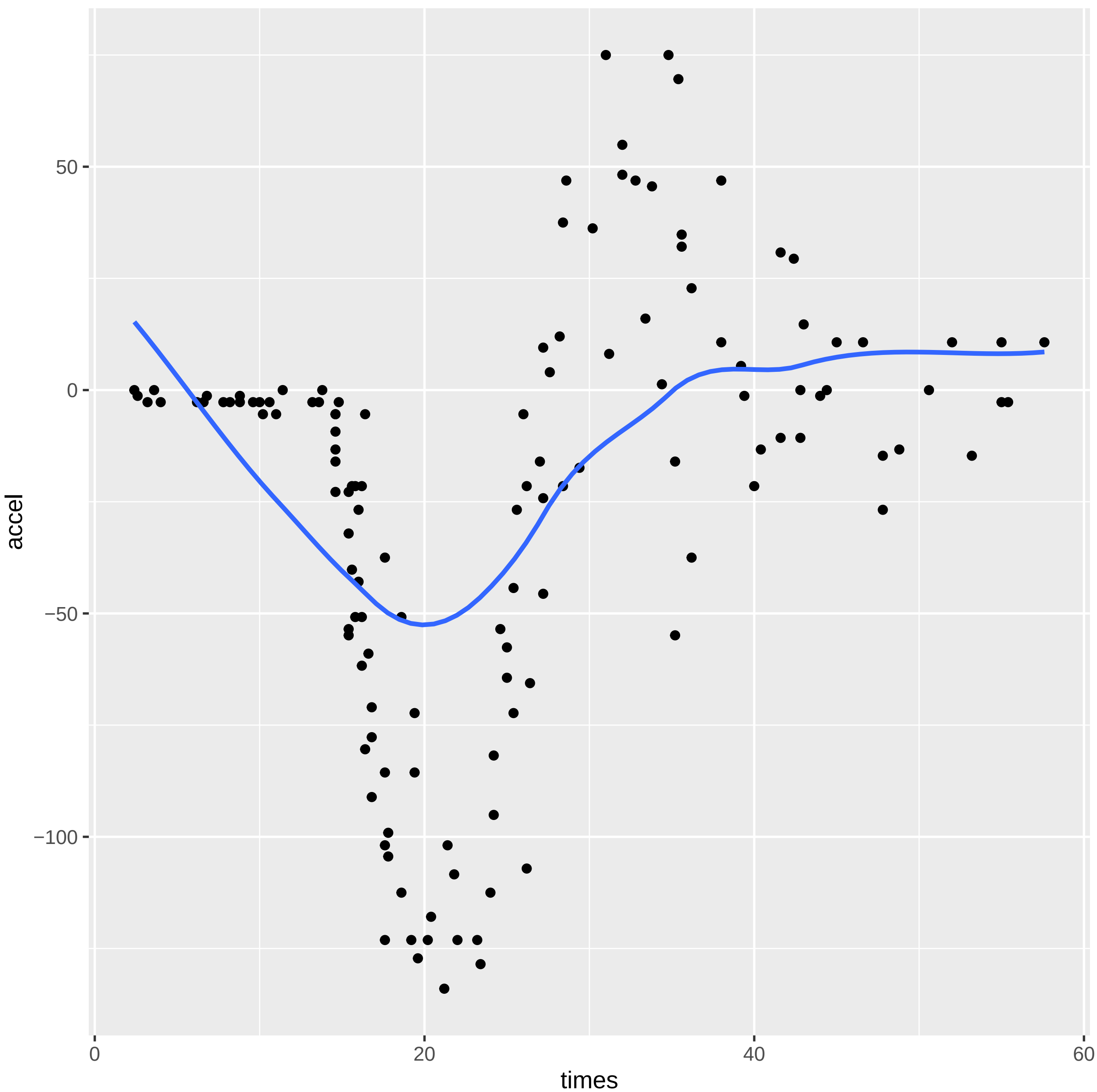


Visually inspecting the models, we believe that the model with degree and span provided the “best” fit.

Part b

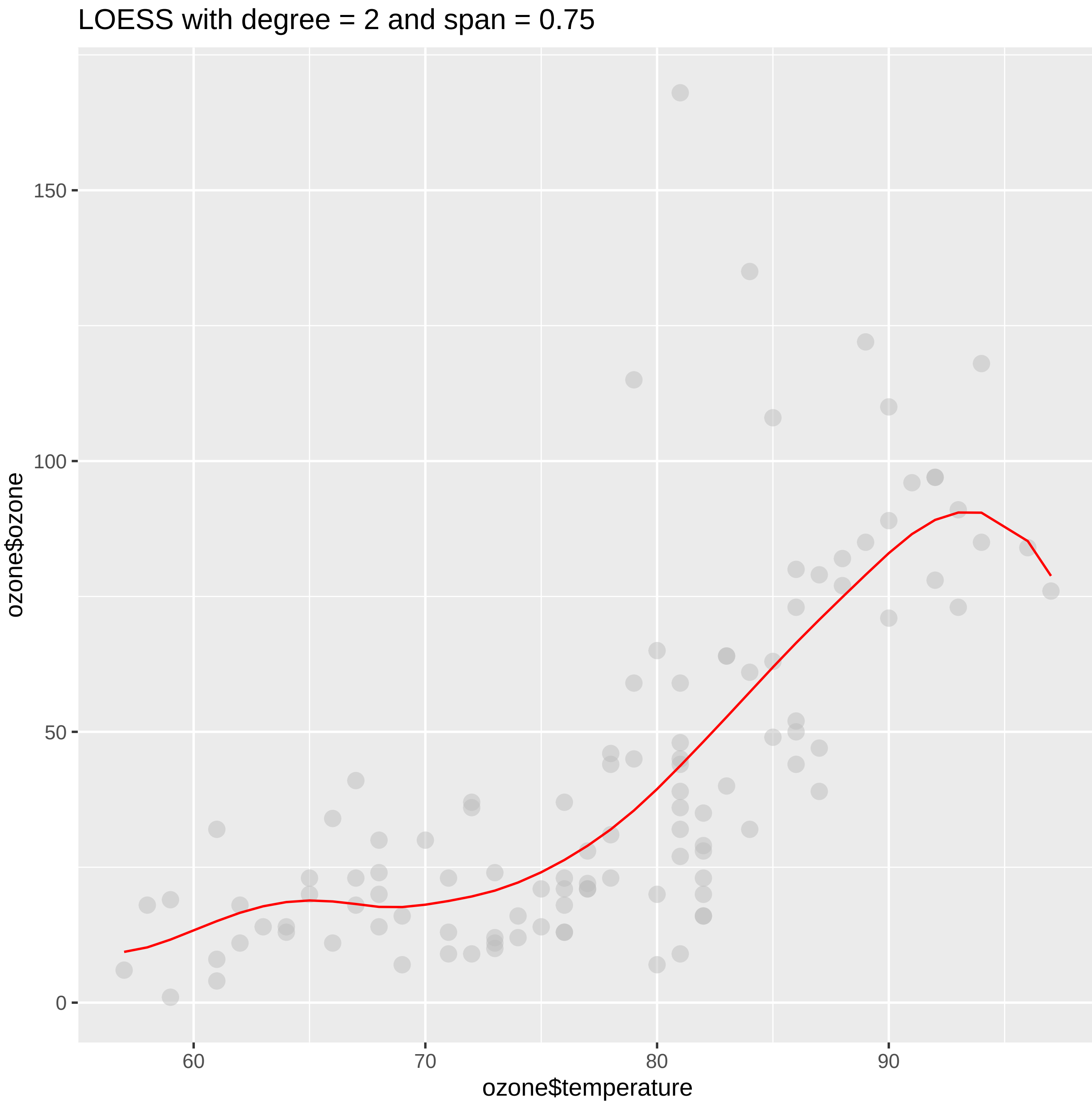
Comparing results with built-in LOESS function

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



The built-in LOESS function results in a fit that does not over-fit the data like our best fits, especially for the fits with degree 2. The model with degree 1 and span 0.4 appears to be the "best" fit.

```
myfit <- myloess(ozone$temperature, ozone$ozone, span = 0.75, degree = 2)
```



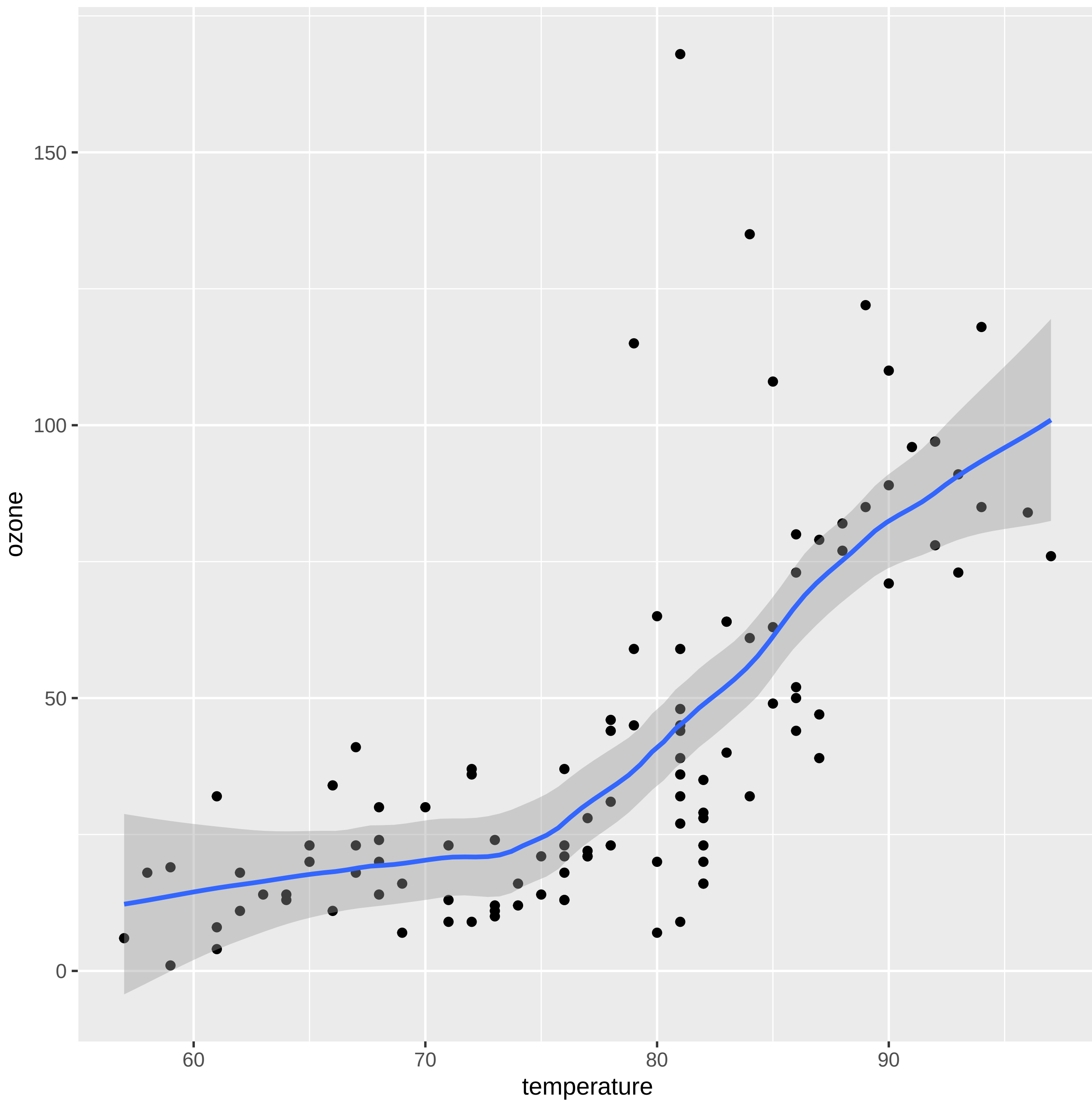

```r
for (i in seq(0.25, 0.75, by = 0.05)) {
  print(loess(ozone ~ temperature, ozone, span = i)$s)
}
```

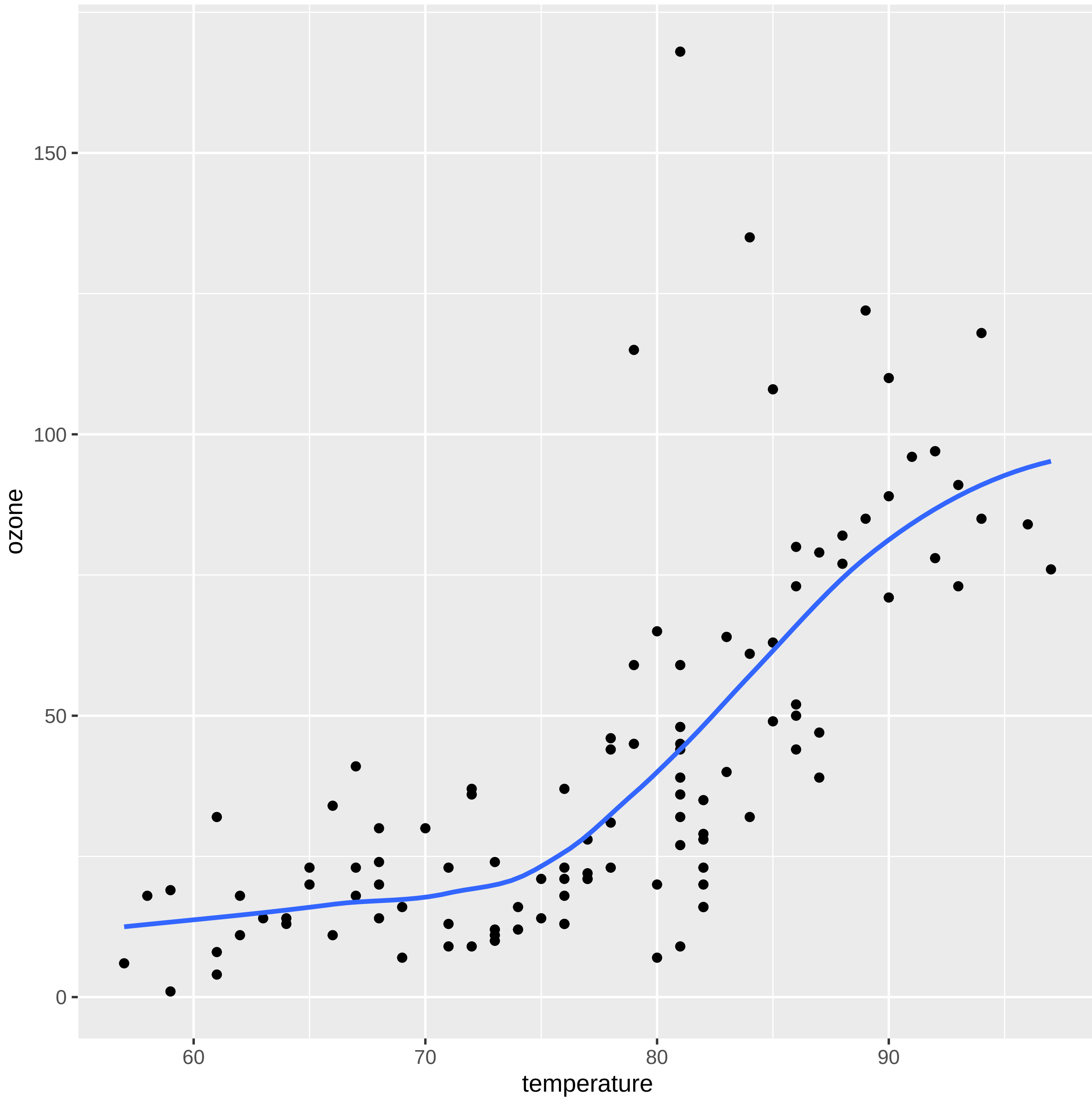
```
[1] 21.35833
[1] 21.68588
[1] 21.67665
[1] 21.83337
[1] 22.12619
[1] 22.19365
[1] 22.27206
[1] 22.33931
[1] 22.36149
[1] 22.35995
[1] 22.35047
```

```r
loess(ozone ~ temperature, ozone, span = 0.75)$fit
```

```
  [1] 16.87755 19.22474 21.14858 14.56757 15.95507 13.32295 14.14456 17.34646
```

```
  [9] 16.47641 17.11209 12.91274 15.46702 16.47641 12.49518 17.11209 14.56757
 [17] 13.32295 19.92519 14.14456 14.14456 16.87755 44.00252 36.17918 25.74618
 [25] 48.23654 81.24996 70.35421 48.23654 28.78253 19.22474 15.95507 19.92519
 [33] 25.74618 57.13432 61.54487 44.00252 52.70108 52.70108 74.42426 86.73008
 [41] 86.73008 78.05206 19.92519 44.00252 39.97026 44.00252 48.23654 57.13432
 [49] 70.35421 61.54487 21.14858 66.00629 61.54487 48.23654 66.00629 74.42426
 [57] 66.00629 52.70108 44.00252 44.00252 44.00252 48.23654 78.05206 81.24996
 [65] 81.24996 66.00629 48.23654 39.97026 28.78253 36.17918 25.74618 32.45702
 [73] 32.45702 28.78253 19.22474 36.17918 44.00252 66.00629 95.21790 91.00772
 [81] 94.10499 91.00772 84.14171 86.73008 89.01782 89.01782 70.35421 57.13432
 [89] 39.97026 32.45702 23.23572 19.92519 44.00252 25.74618 28.78253 18.48044
 [97] 18.48044 32.45702 16.87755 25.74618 17.11209 48.23654 15.46702 18.48044
[105] 44.00252 17.34646 15.00645 17.74710 23.23572 25.74618 17.11209
```





150
100
50
0
ozone
60
70
80
90
temperature