

HW2.2_Mary_Futey

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Air Quality dataset

- Convert date and time to factor, check for NAs, switch comma to decimal

```
airq <- read.csv("/Users/maryfutey/desktop/AirQualityUCI/AirQualityUCI.csv",
                header = TRUE,
                dec=",")
#deleted column NMHC.GT. as there were many "-200" values
airq <- airq[, -5]

summary(airq)
```

```
##           Date           Time           CO.GT.           PT08.S1.CO.
## 01/01/2005: 24  00.00.00: 390  Min.    :-200.00  Min.    :-200
## 01/02/2005: 24  01.00.00: 390  1st Qu.:   0.60  1st Qu.: 921
## 01/03/2005: 24  02.00.00: 390  Median :   1.50  Median :1053
## 01/04/2004: 24  03.00.00: 390  Mean     :-34.21  Mean     :1049
## 01/04/2005: 24  04.00.00: 390  3rd Qu.:   2.60  3rd Qu.:1221
## 01/05/2004: 24  05.00.00: 390  Max.     : 11.90  Max.     :2040
## (Other)      :9213  (Other) :7017
##      C6H6.GT.      PT08.S2.NMHC.      NOx.GT.      PT08.S3.NOx.
## Min.    :-200.000  Min.    :-200.0  Min.    :-200.0  Min.    :-200
## 1st Qu.:   4.000  1st Qu.: 711.0  1st Qu.:  50.0  1st Qu.: 637
## Median :   7.900  Median : 895.0  Median : 141.0  Median : 794
## Mean     :   1.866  Mean     : 894.6  Mean     : 168.6  Mean     : 795
## 3rd Qu.:  13.600  3rd Qu.:1105.0  3rd Qu.: 284.0  3rd Qu.: 960
## Max.     :  63.700  Max.     :2214.0  Max.     :1479.0  Max.     :2683
##
##      NO2.GT.      PT08.S4.NO2.      PT08.S5.O3.      T
## Min.    :-200.00  Min.    :-200  Min.    :-200.0  Min.    :-200.000
## 1st Qu.:  53.00  1st Qu.:1185  1st Qu.: 700.0  1st Qu.: 10.900
## Median :  96.00  Median :1446  Median : 942.0  Median : 17.200
## Mean     :  58.15  Mean     :1391  Mean     : 975.1  Mean     :  9.778
## 3rd Qu.: 133.00  3rd Qu.:1662  3rd Qu.:1255.0  3rd Qu.: 24.100
## Max.     : 340.00  Max.     :2775  Max.     :2523.0  Max.     : 44.600
##
##           RH           AH
## Min.    :-200.00  Min.    :-200.0000
## 1st Qu.:  34.10  1st Qu.:   0.6923
## Median :  48.60  Median :   0.9768
## Mean     :  39.49  Mean     : -6.8376
## 3rd Qu.:  61.90  3rd Qu.:   1.2962
## Max.     :  88.70  Max.     :   2.2310
```

```
##
```

```
airq_long <- gather(airq, key="measurement", value="value", -c(Date,Time))
```

```
airq_long$Date <- as.factor(airq_long$Date)
```

```
airq_long$Time <- as.factor(airq_long$Time)
```

```
airq_long$measurement <- as.factor(airq_long$measurement)
```

- Clean and remove "-200" values as they are not possible / erroneous

```
airq_fil <- airq_long %>%  
  filter(value != -200)
```

```
summary(airq_fil)
```

```
##          Date          Time          measurement          value  
## 02/04/2005: 288 09.00.00: 4396 AH : 8991 Min. : -1.9  
## 03/04/2005: 288 10.00.00: 4392 C6H6.GT. : 8991 1st Qu.: 13.2  
## 15/03/2005: 288 12.00.00: 4389 PT08.S1.CO. : 8991 Median : 135.0  
## 16/03/2005: 288 13.00.00: 4385 PT08.S2.NMHC.: 8991 Mean : 496.4  
## 18/03/2005: 288 11.00.00: 4378 PT08.S3.NOx. : 8991 3rd Qu.: 948.0  
## 19/03/2005: 288 05.00.00: 4376 PT08.S4.NO2. : 8991 Max. : 2775.0  
## (Other) :102298 (Other) :77710 (Other) :50080
```

```
colSums(is.na(airq_fil))
```

```
##          Date          Time measurement          value  
##          0          0          0          0
```

- Need to normalize data

```
airq_wide <- spread(airq_fil, key = "measurement", value = "value")  
airq_wide <- na.omit(airq_wide)
```

```
norm <- function(x) {  
  (x - min(x)) / (max(x) - min(x))  
}
```

```
airq_norm <- as.data.frame(lapply(airq_wide[3:14], norm))
```

```
airq_norm$Date <- airq_wide$Date
```

```
airq_norm$Time <- airq_wide$Time
```

```
airq_norm_long <- gather(airq_norm, key = "measurement", value = "value", -c(Date, Time))
```

```
#Explore multicollinearity
```

```
*Choose good predictors
```

```
*Check residuals
```

```
*Do you need some non-linear transformations for some of predictors? Or maybe response? +log(x) +sqrt(x)  
+(x)^2
```

```
** selected two predictor with high R2, but non-linear tp transform: PT08.S2.NMHC.
```

```
# PT08.S2.NMHC.: residuals look better after quadratic transformation,
```

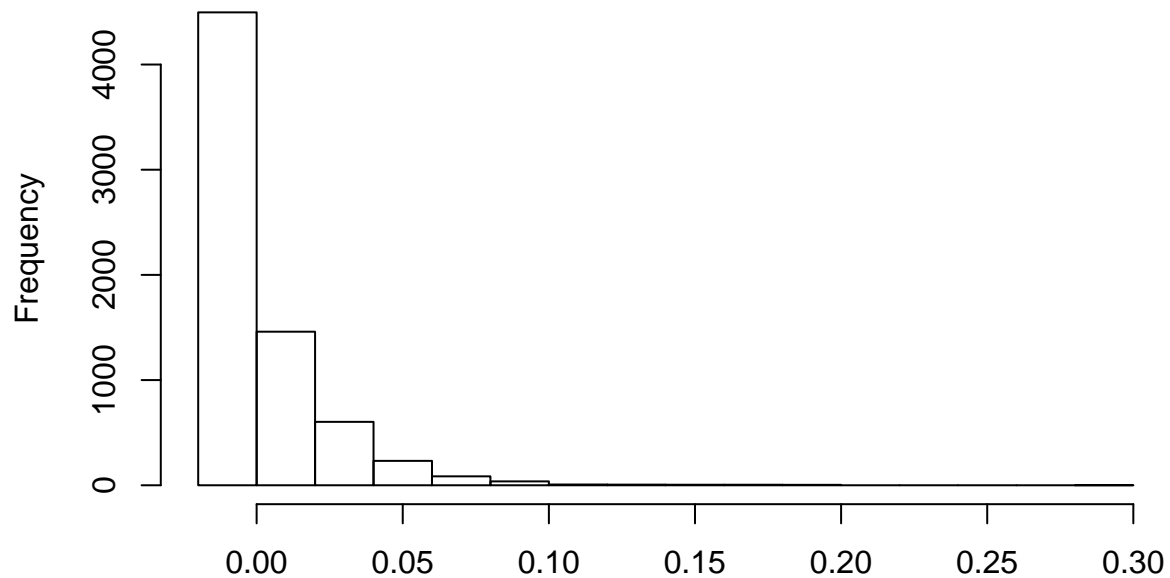
```
#however residuals vs fitted plot cubic
```

```
# R2 of 0.999, how so high?
```

```
lm_3 <- lm(C6H6.GT. ~ PT08.S2.NMHC., airq_norm)
```

```
residuals(lm_3) %>% hist(main = "residuals PT08.S2.NMHC.")
```

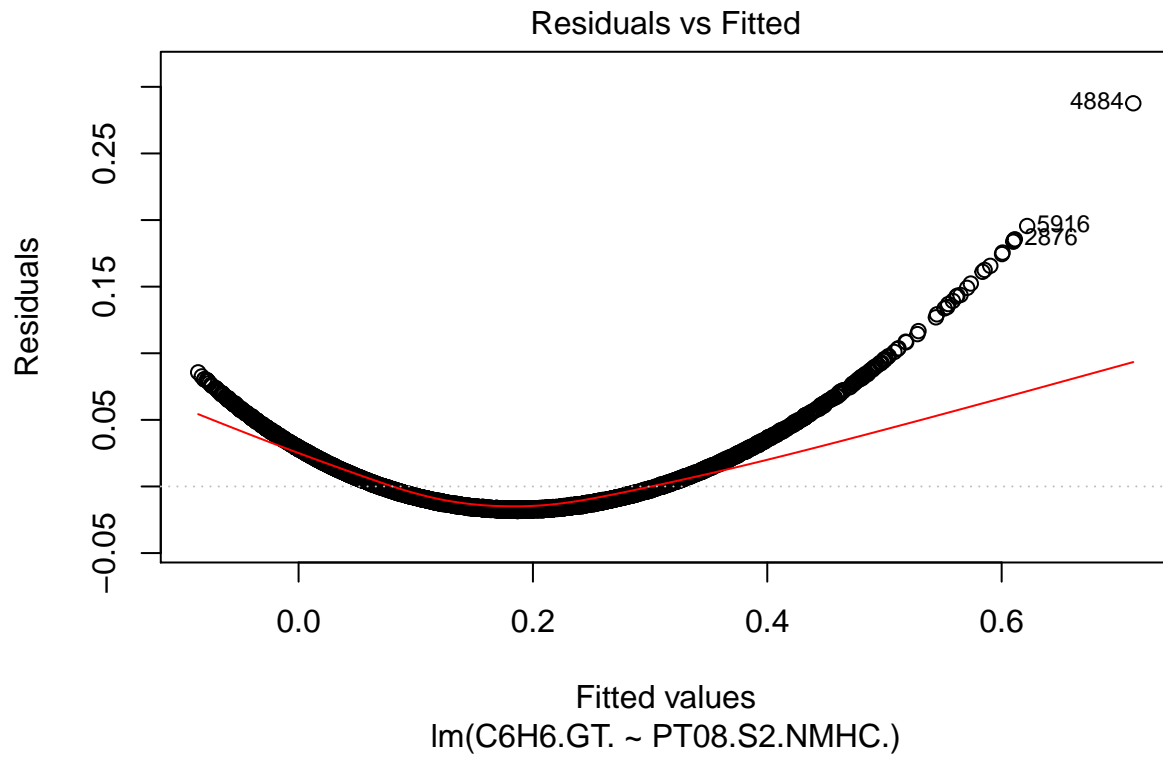
residuals PT08.S2.NMHC.



```
summary(lm_3)
```

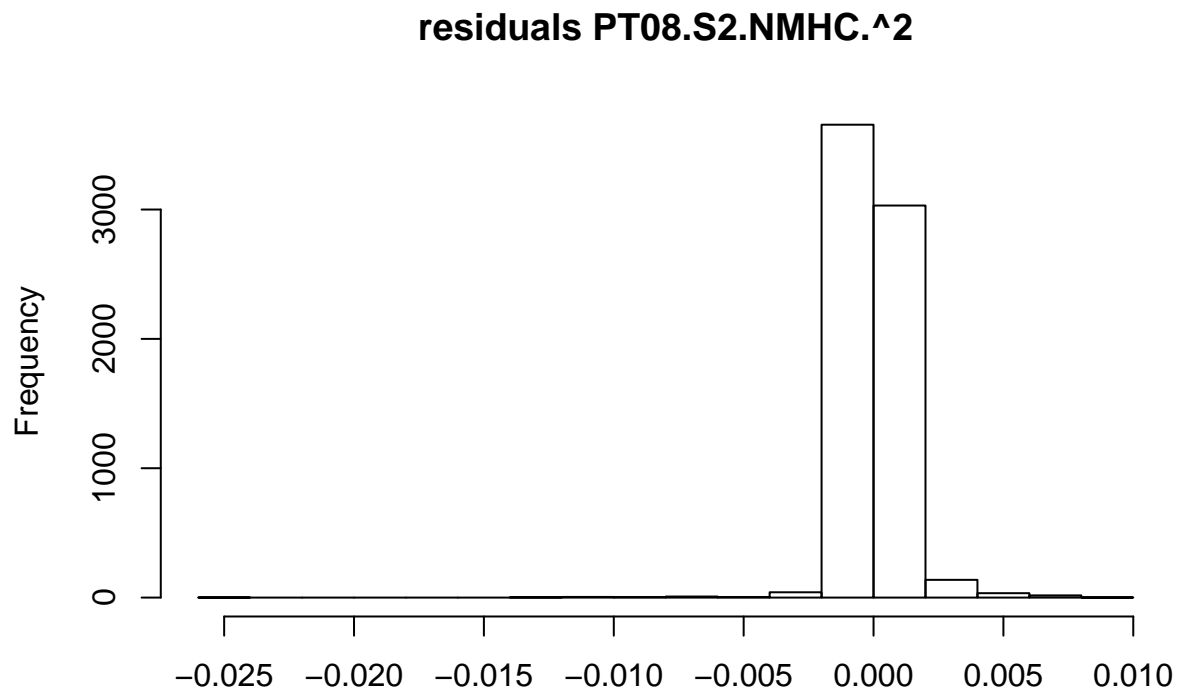
```
##
## Call:
## lm(formula = C6H6.GT. ~ PT08.S2.NMHC., data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.018385 -0.015140 -0.007871  0.007973  0.287650
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.0856861  0.0006204  -138.1   <2e-16 ***
## PT08.S2.NMHC.  0.7980363  0.0018053   442.1   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.02177 on 6939 degrees of freedom
## Multiple R-squared:  0.9657, Adjusted R-squared:  0.9657
## F-statistic: 1.954e+05 on 1 and 6939 DF, p-value: < 2.2e-16
```

```
plot(lm_3, which = 1)
```



```
airq_norm$NMHC_sq <- (airq_norm$PT08.S2.NMHC.)^2

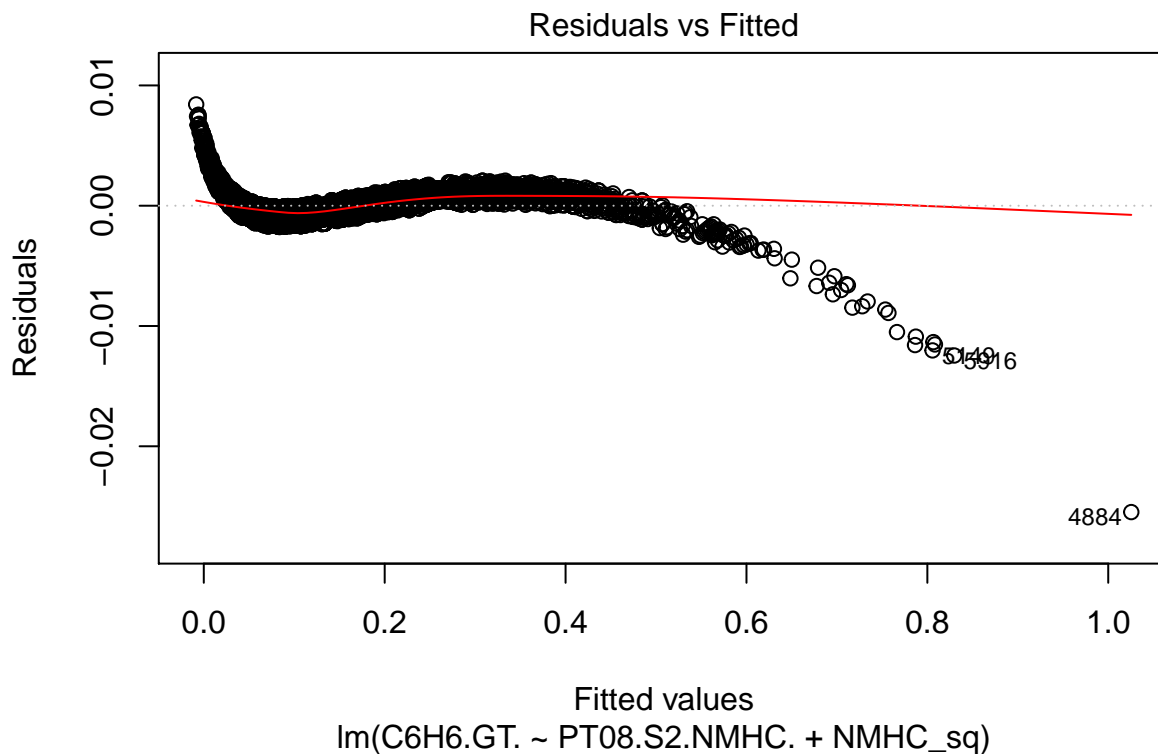
lm_4 <- lm(C6H6.GT. ~ PT08.S2.NMHC. + NMHC_sq, airq_norm)
residuals(lm_4) %>% hist(main = "residuals PT08.S2.NMHC.^2")
```



```
summary(lm_4)
```

```
##
## Call:
## lm(formula = C6H6.GT. ~ PT08.S2.NMHC. + NMHC_sq, data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0254697 -0.0007130 -0.0000817  0.0006329  0.0084216
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -8.422e-03  6.223e-05  -135.3   <2e-16 ***
## PT08.S2.NMHC.  2.550e-01  3.773e-04   675.8   <2e-16 ***
## NMHC_sq       7.789e-01  5.217e-04  1493.0   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.001213 on 6938 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
## F-statistic: 3.26e+07 on 2 and 6938 DF,  p-value: < 2.2e-16
```

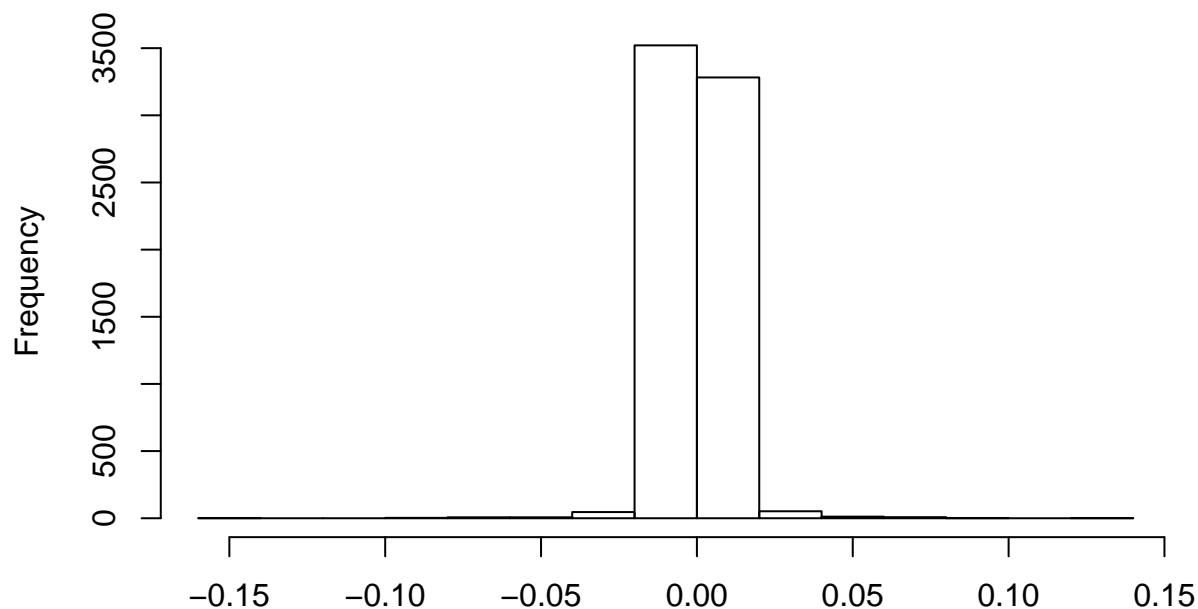
```
plot(lm_4, which = 1)
```



```
airq_norm$NMHC_rt <- sqrt(airq_norm$PT08.S2.NMHC.)
```

```
lm_2 <- lm(C6H6.GT. ~ PT08.S2.NMHC. + NMHC_rt, airq_norm)
residuals(lm_2) %>% hist(main = "residuals PT08.S2.NMHC. sqrt transformed")
```

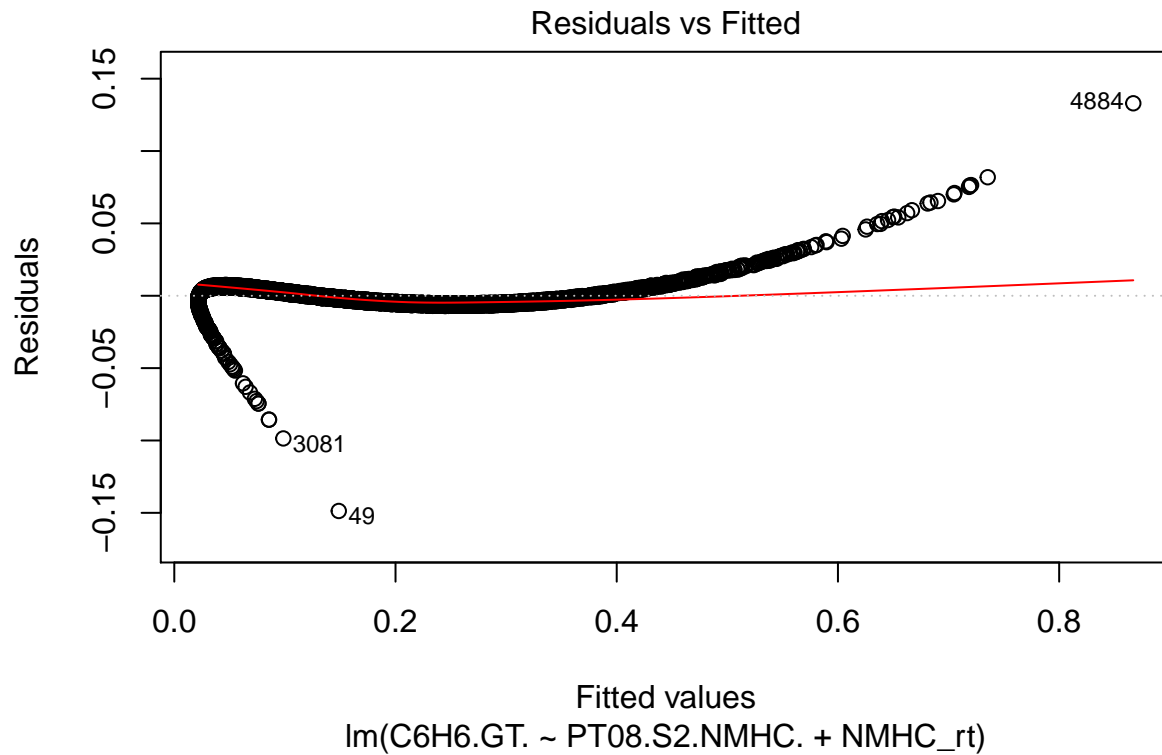
residuals PT08.S2.NMHC. sqrt transformed



```
summary(lm_2)
```

```
##
## Call:
## lm(formula = C6H6.GT. ~ PT08.S2.NMHC. + NMHC_rt, data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.148700 -0.004664 -0.000351  0.004615  0.132983
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   0.148700   0.001115   133.3  <2e-16 ***
## PT08.S2.NMHC.  1.628181   0.003924   414.9  <2e-16 ***
## NMHC_rt       -0.909864   0.004241  -214.5  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.00788 on 6938 degrees of freedom
## Multiple R-squared:  0.9955, Adjusted R-squared:  0.9955
## F-statistic: 7.688e+05 on 2 and 6938 DF,  p-value: < 2.2e-16
```

```
plot(lm_2, which = 1)
```



Make a coorelation matrix to select predictors to use in multiple linear regression

- due to deletion of NHMC column, matrix is differnet from the previous homework

```
airq_sub <- airq_norm[, 1:12]
colnames(airq_sub) <- c(
  "Abs H",
  "C6H6",
  "CO",
  "NO2",
  "NOx",
  "S1.CO",
  "S2.NMHC",
  "S3.NOx",
  "S4.NO2",
  "S5.O3",
  "Rel H",
  "Temp"
)

airq_cor <- round(cor(airq_sub, method = "kendall"),2)

#reorder, create upper triangle
reorder_airq_cor <- function(airq_cor){
  # Use correlation between variables as distance
  dd <- as.dist((1-airq_cor)/2)
  hc <- hclust(dd)
  airq_cor <-airq_cor[hc$order, hc$order]
}
```

```

get_upper_tri <- function(airq_cor){
  airq_cor[lower.tri(airq_cor)]<- NA
  return(airq_cor)
}

airq_cor <- reorder_airq_cor(airq_cor)
upper_tri <- get_upper_tri(airq_cor)
melt_uppertri <- melt(upper_tri, na.rm = TRUE)

```

Warning in melt(upper_tri, na.rm = TRUE): The melt generic in data.table has
 ## been passed a matrix and will attempt to redirect to the relevant reshape2
 ## method; please note that reshape2 is deprecated, and this redirection is now
 ## deprecated as well. To continue using melt methods from reshape2 while both
 ## libraries are attached, e.g. melt.list, you can prepend the namespace like
 ## reshape2::melt(upper_tri). In the next version, this warning will become an
 ## error.

```

p1 <- ggplot(melt_uppertri,
             aes(Var2, Var1,
                 fill = value)) +
  geom_tile(color = "white") +
  scale_fill_gradient2(low = "blue", high = "red", mid = "white",
                      midpoint = 0, limit = c(-1,1), space = "Lab",
                      name="Kendall\nCorrelation") +
  ggtitle("Correlation Matrix for Air Quality Dataset") +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, vjust = 1,
                                    size = 7, hjust = 1)) +

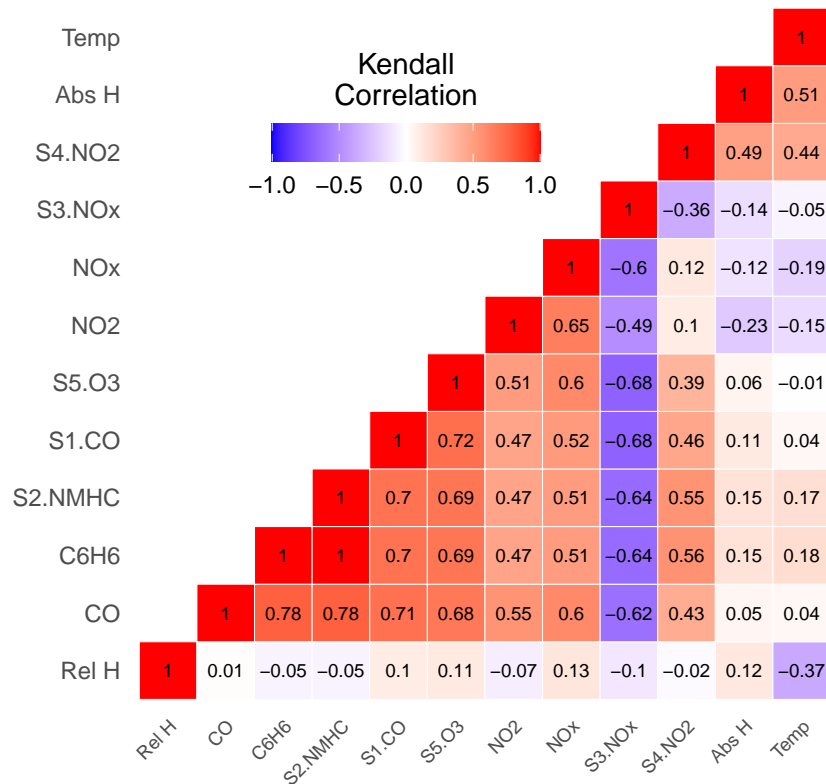
  coord_fixed() +
  geom_text(aes(Var2,
                Var1,
                label = value),
            color = "black", size = 2.6) +

  theme(
    axis.title.x = element_blank(),
    axis.title.y = element_blank(),
    panel.grid.major = element_blank(),
    panel.border = element_blank(),
    panel.background = element_blank(),
    axis.ticks = element_blank(),
    legend.justification = c(1, 0),
    legend.position = c(0.6, 0.7),
    legend.direction = "horizontal")+
  guides(fill = guide_colorbar(barwidth = 7, barheight = 1,
                              title.position = "top", title.hjust = 0.5))

```

p1

Correlation Matrix for Air Quality Dataset

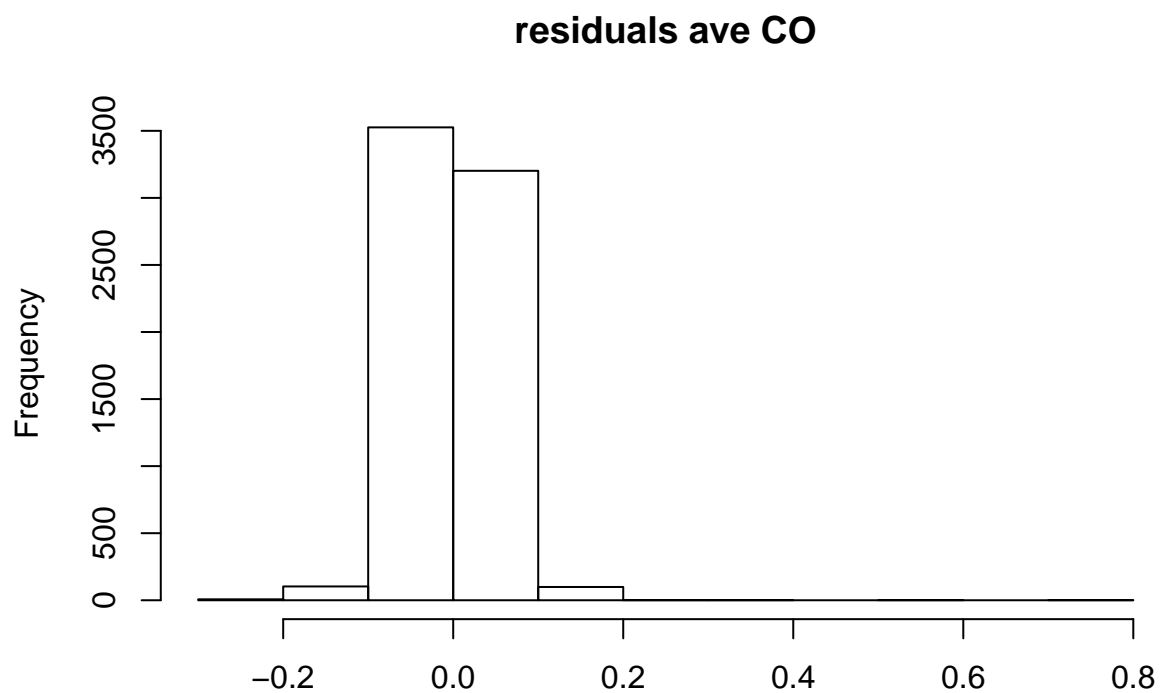


#single linear regression with good predictor for baseline comparison

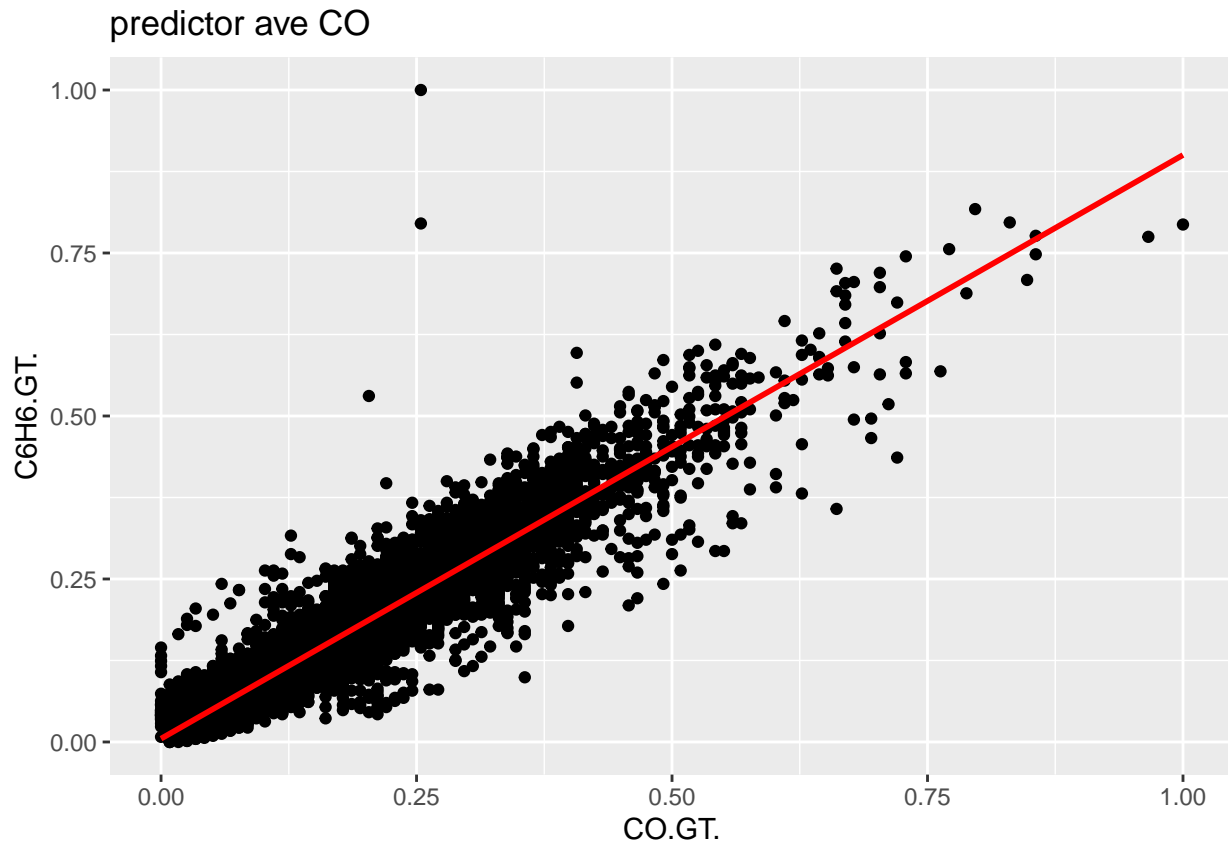
```
lm_5 <- lm(C6H6.GT. ~ CO.GT., airq_norm)
summary(lm_5)
```

```
##
## Call:
## lm(formula = C6H6.GT. ~ CO.GT., data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.23935 -0.02496 -0.00249  0.02357  0.76733
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.0050753  0.0009115   5.568 2.67e-08 ***
## CO.GT.       0.8952134  0.0042471 210.782 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.04321 on 6939 degrees of freedom
## Multiple R-squared:  0.8649, Adjusted R-squared:  0.8649
## F-statistic: 4.443e+04 on 1 and 6939 DF, p-value: < 2.2e-16
```

```
residuals(lm_5) %>% hist(main = "residuals ave CO")
```



```
ggplot(lm_5,  
  aes(x = CO.GT., y = C6H6.GT.)) +  
  geom_point() +  
  geom_line(aes(y = .fitted), color = "red", size = 1) +  
  ggtitle("predictor ave CO")
```



selected the following predictors: CO.GT., PT08.S1.CO. and PT08.S2.NMHC. for building a model

```
#CO: corr 0.88, good residuals, high R2, sigif, linear
#PT08.S1.CO., corr 0.83, residuals okay, high R2, sigif, linear
#PT08.S2.NMHC., sym residuals, high R2, sigif, linear

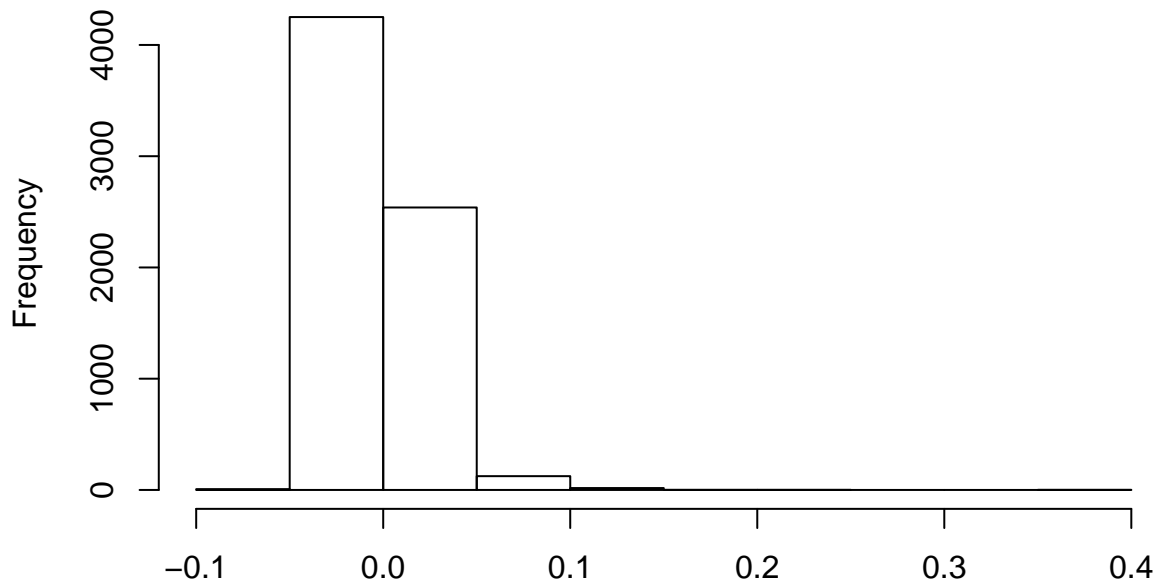
#very high R2, but residuals vs fitted plot not linear

lm_6 <- lm(C6H6.GT. ~ CO.GT. + PT08.S1.CO. + PT08.S2.NMHC., airq_norm)
summary(lm_6)
```

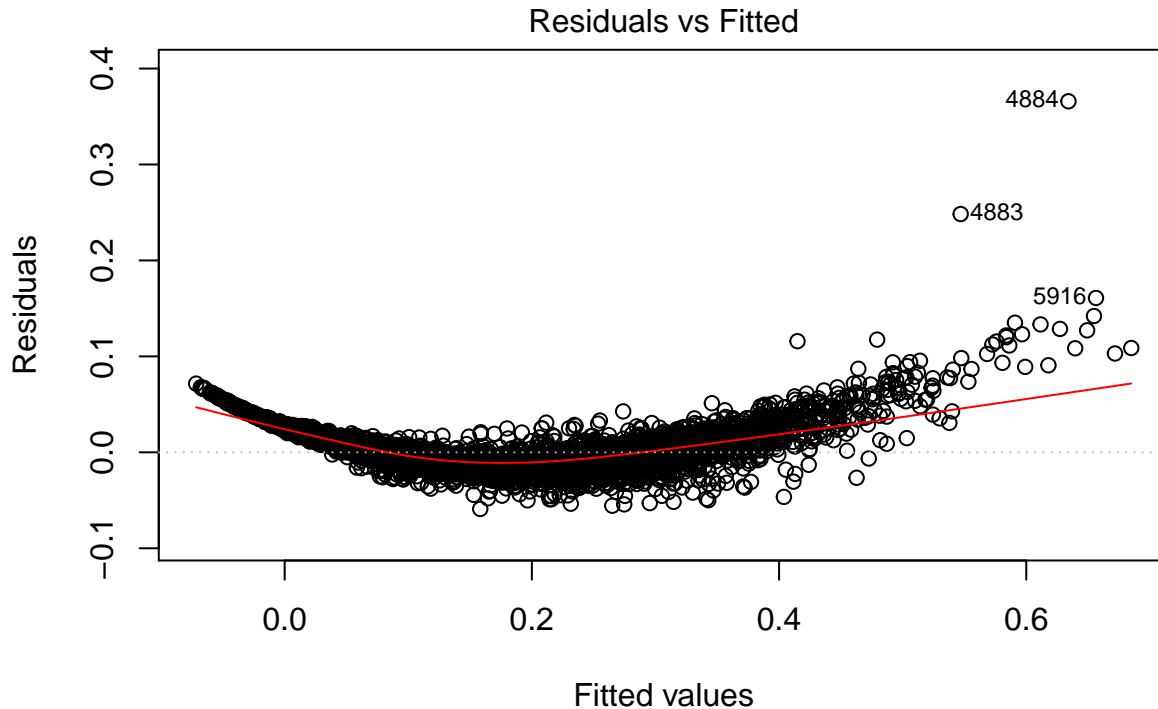
```
##
## Call:
## lm(formula = C6H6.GT. ~ CO.GT. + PT08.S1.CO. + PT08.S2.NMHC.,
##     data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.05902 -0.01174 -0.00468  0.00846  0.36586
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.072055   0.000688  -104.737 < 2e-16 ***
## CO.GT.        0.197796   0.005113   38.683 < 2e-16 ***
## PT08.S1.CO.   -0.024579   0.003475   -7.073 1.66e-12 ***
```

```
## PT08.S2.NMHC. 0.669088 0.004471 149.644 < 2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.01969 on 6937 degrees of freedom
## Multiple R-squared: 0.972, Adjusted R-squared: 0.972
## F-statistic: 8.016e+04 on 3 and 6937 DF, p-value: < 2.2e-16
residuals(lm_6) %>% hist(main = "residuals multi regression 3 predictors and S2.NMHC transformed")
```

residuals multi regression 3 predictors and S2.NMHC transformed



```
plot(lm_6, which = 1)
```



lm(C6H6.GT. ~ CO.GT. + PT08.S1.CO. + PT08.S2.NMHC.)

```
#CO: corr 0.88, good residuals, high R2, sigif, linear
#PT08.S1.CO., corr 0.83, residuals okay, high R2, sigif, linear
#PT08.S2.NMHC., sym residuals, high R2, sigif, linear
```

```
#inclusion of transformed PT08.S2.NMHC appears to make residuals vs fitted plot cubic?
```

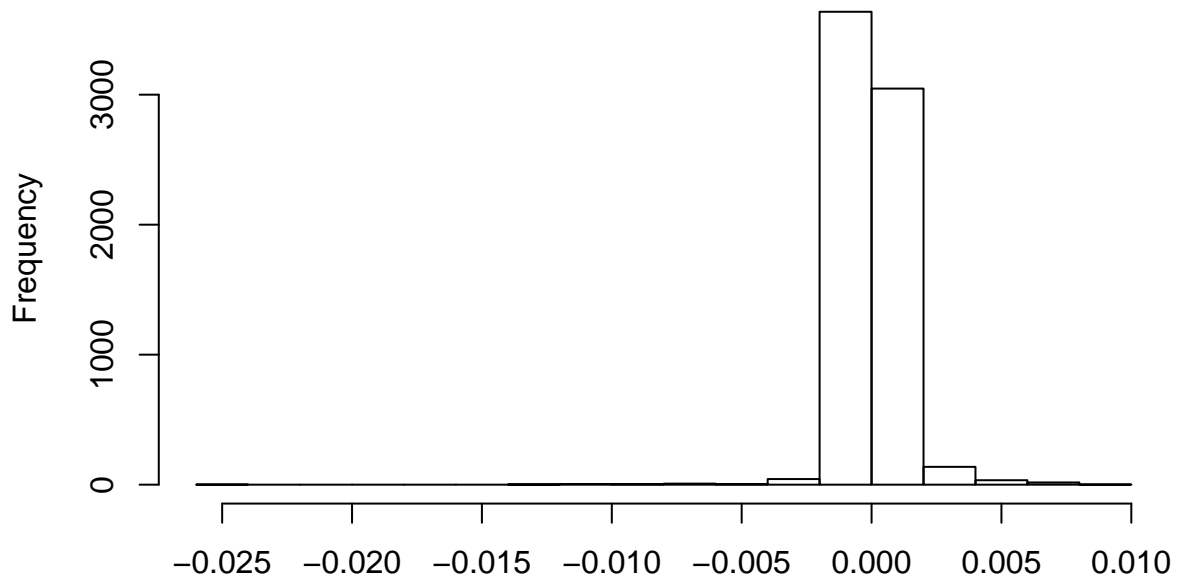
```
lm_6 <- lm(C6H6.GT. ~ CO.GT. + PT08.S1.CO. + PT08.S2.NMHC. + NMHC_sq, airq_norm)
summary(lm_6)
```

```
##
## Call:
## lm(formula = C6H6.GT. ~ CO.GT. + PT08.S1.CO. + PT08.S2.NMHC. +
##     NMHC_sq, data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0240720 -0.0007106 -0.0000823  0.0006286  0.0084289
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -8.471e-03  6.321e-05 -134.011 < 2e-16 ***
## CO.GT.         1.430e-03  3.461e-04   4.133 3.63e-05 ***
## PT08.S1.CO.    5.964e-04  2.143e-04   2.783  0.0054 **
## PT08.S2.NMHC.  2.542e-01  4.117e-04  617.324 < 2e-16 ***
## NMHC_sq       7.777e-01  5.748e-04 1353.018 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.00121 on 6936 degrees of freedom
## Multiple R-squared:  0.9999, Adjusted R-squared:  0.9999
```

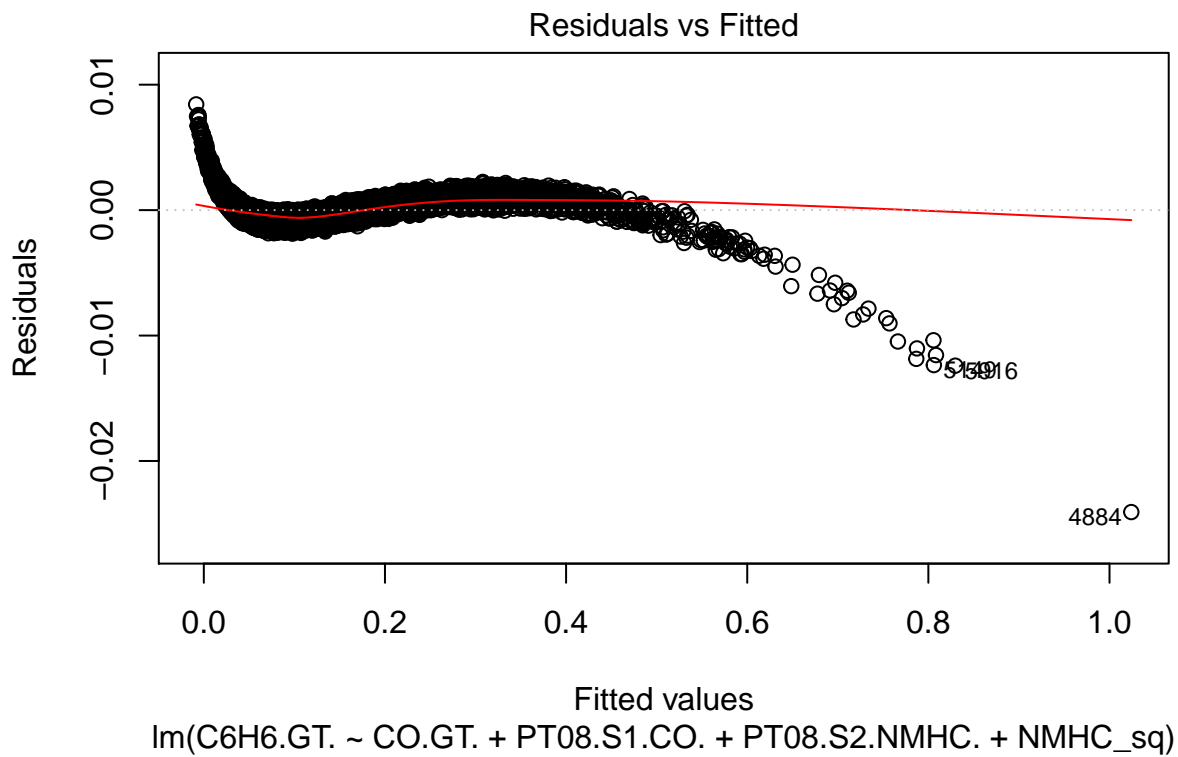
```
## F-statistic: 1.638e+07 on 4 and 6936 DF, p-value: < 2.2e-16
```

```
residuals(lm_6) %>% hist(main = "residuals multi regression 3 predictors and S2.NMHC transformed")
```

residuals multi regression 3 predictors and S2.NMHC transformed



```
plot(lm_6, which = 1)
```

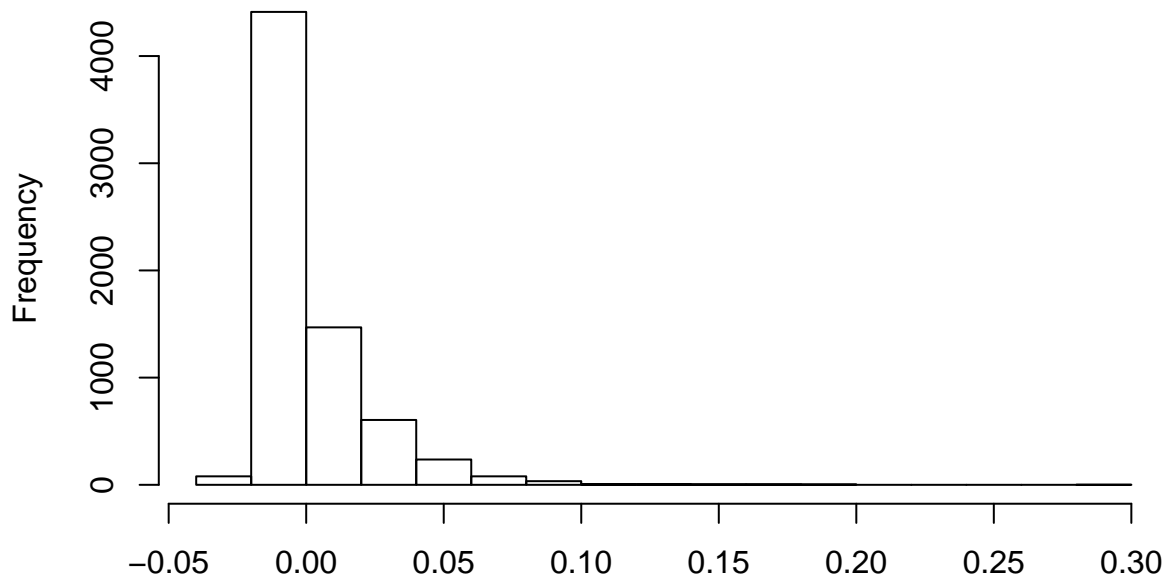


Model with the following predictors: PT08.S1.CO. and PT08.S2.NMHC.

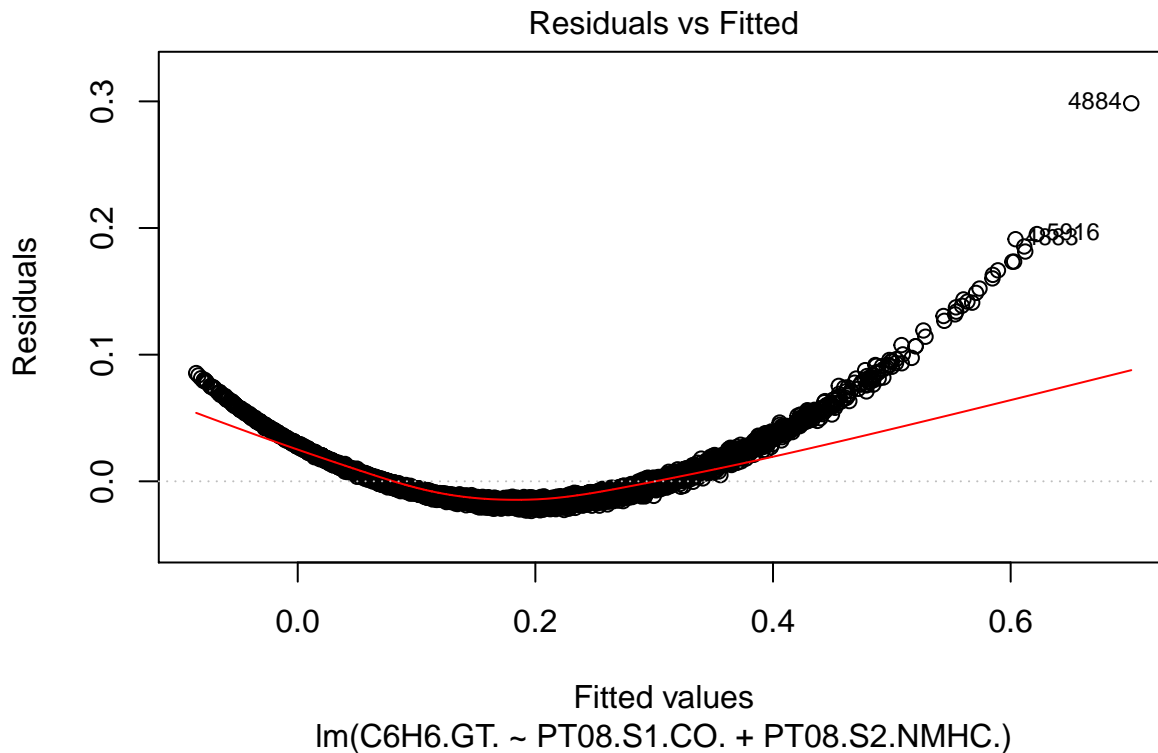
```
# residuals vs fitted plot is not linear
lm_7 <- lm(C6H6.GT. ~ PT08.S1.CO. + PT08.S2.NMHC., airq_norm)
summary(lm_7)

##
## Call:
## lm(formula = C6H6.GT. ~ PT08.S1.CO. + PT08.S2.NMHC., data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.023401 -0.014539 -0.007786  0.008009  0.298478
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.0866162  0.0006349 -136.429 < 2e-16 ***
## PT08.S1.CO.    0.0232981  0.0035798   6.508 8.14e-11 ***
## PT08.S2.NMHC.  0.7756448  0.0038829 199.760 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.02171 on 6938 degrees of freedom
## Multiple R-squared:  0.9659, Adjusted R-squared:  0.9659
## F-statistic: 9.831e+04 on 2 and 6938 DF, p-value: < 2.2e-16
residuals(lm_7) %>% hist(main = "residuals multi PT08.S1.CO. + PT08.S2.NMHC. predictors")
```

residuals multi PT08.S1.CO. + PT08.S2.NMHC. predictors



```
plot(lm_7, which = 1)
```



```
# variance inflation factor:
#how much the variance of a coefficient is inflated due to multicollinearity
#vif <5, which is good, however based on the plots and residuals,
# am not selecting this model as the "final" model
vif(lm_7)
```

```
##    PT08.S1.CO. PT08.S2.NMHC.
##      4.653696      4.653696
```

Model with CO.GT.and PT08.S2.NMHC.

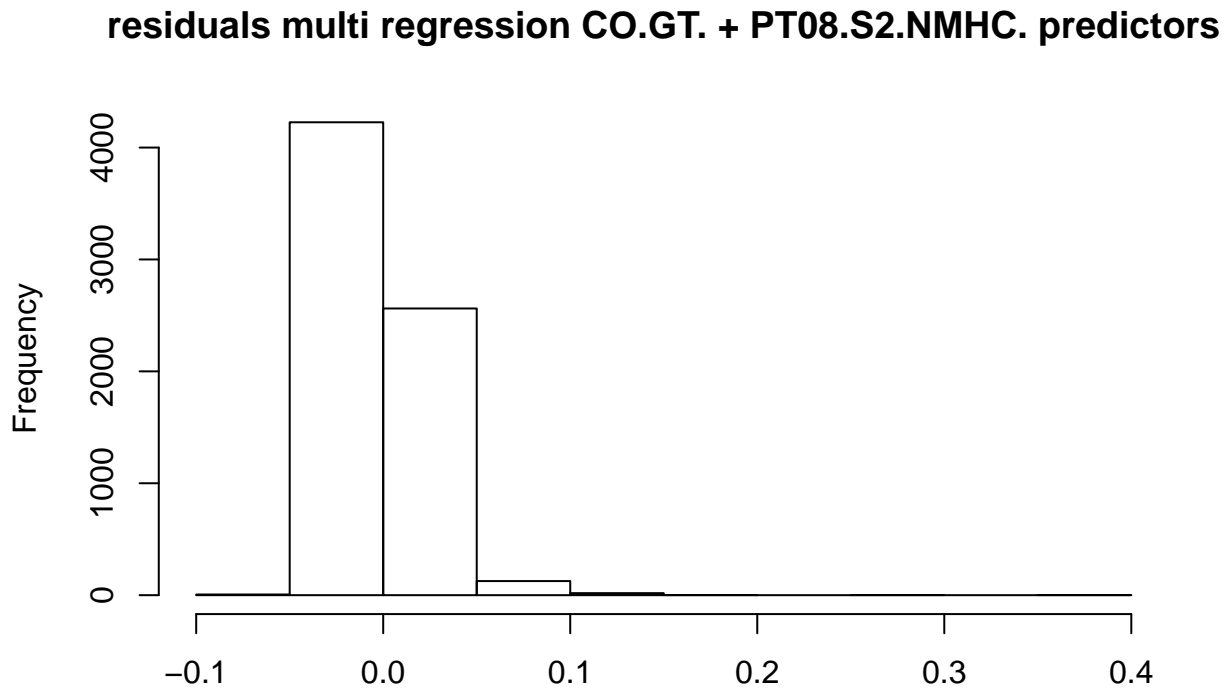
```
# seems to be quadratic, also built a model with PT08.S2.NMHC.^2, however did not improve the model
```

```
lm_8 <- lm(C6H6.GT. ~ CO.GT. + PT08.S2.NMHC., airq_norm)
summary(lm_8)
```

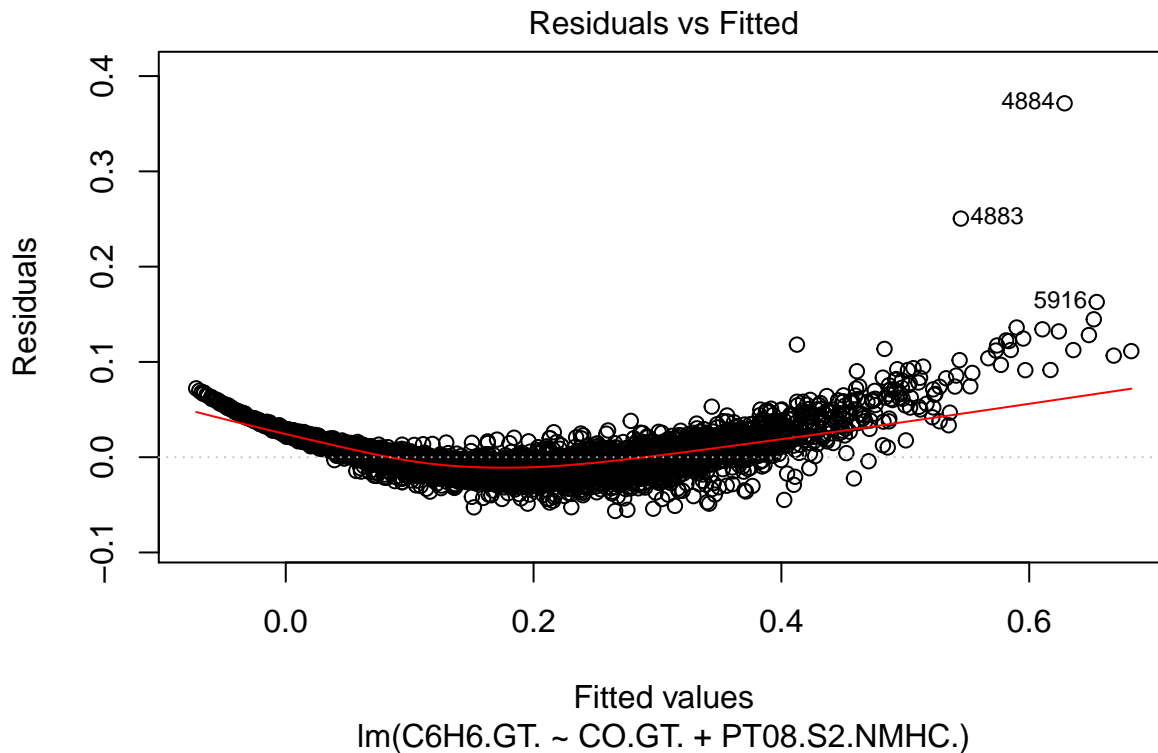
```
##
## Call:
## lm(formula = C6H6.GT. ~ CO.GT. + PT08.S2.NMHC., data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.05643 -0.01185 -0.00467  0.00841  0.37145
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.0738605  0.0006411  -115.20  <2e-16 ***
## CO.GT.         0.1849137  0.0047948   38.56  <2e-16 ***
## PT08.S2.NMHC.  0.6554025  0.0040451  162.02  <2e-16 ***
## ---
```



```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.01976 on 6938 degrees of freedom
## Multiple R-squared:  0.9718, Adjusted R-squared:  0.9718
## F-statistic: 1.194e+05 on 2 and 6938 DF,  p-value: < 2.2e-16
residuals(lm_8) %>% hist(main = "residuals multi regression CO.GT. + PT08.S2.NMHC. predictors")
```



```
plot(lm_8, which = 1)
```



```
# vif >5: indicates multicollinearity
vif(lm_8)
```

```
##          CO.GT. PT08.S2.NMHC.
##          6.096192      6.096192
```

Final model with the following predictors: CO.GT.and PT08.S1.CO.

```
# predictors significant, best residuals with a few outliers on plot,
# high R2 (larger than single regression with CO) and low vif
```

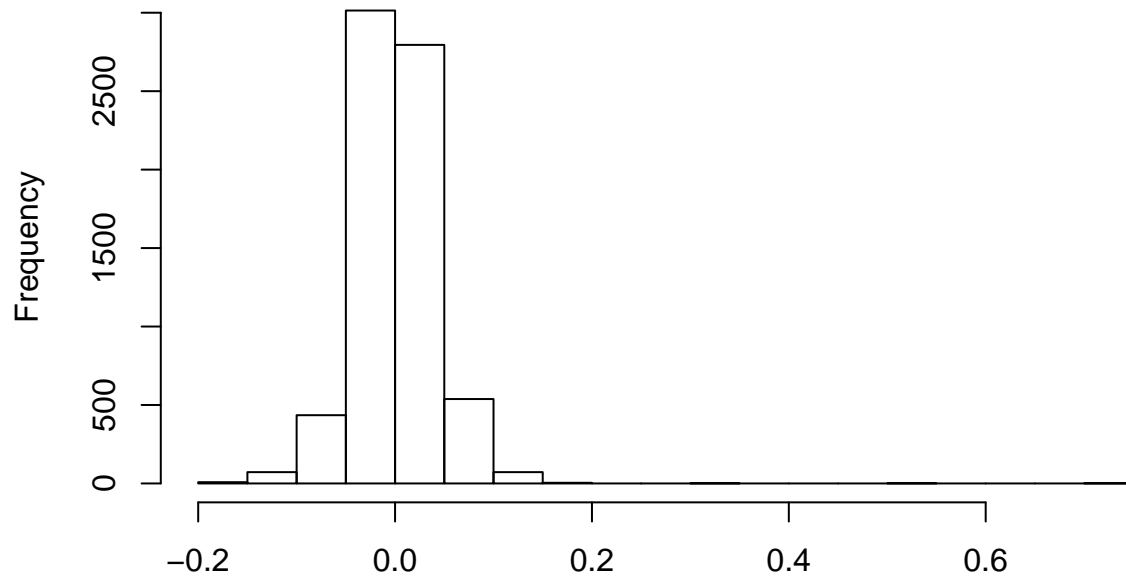
```
lm_9 <- lm(C6H6.GT. ~ CO.GT. + PT08.S1.CO., airq_norm)
summary(lm_9)
```

```
##
## Call:
## lm(formula = C6H6.GT. ~ CO.GT. + PT08.S1.CO., data = airq_norm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.19287 -0.02482 -0.00104  0.02346  0.74546
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -0.023085   0.001244  -18.55  <2e-16 ***
## CO.GT.       0.669212   0.008281   80.81  <2e-16 ***
## PT08.S1.CO.  0.200433   0.006441   31.12  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

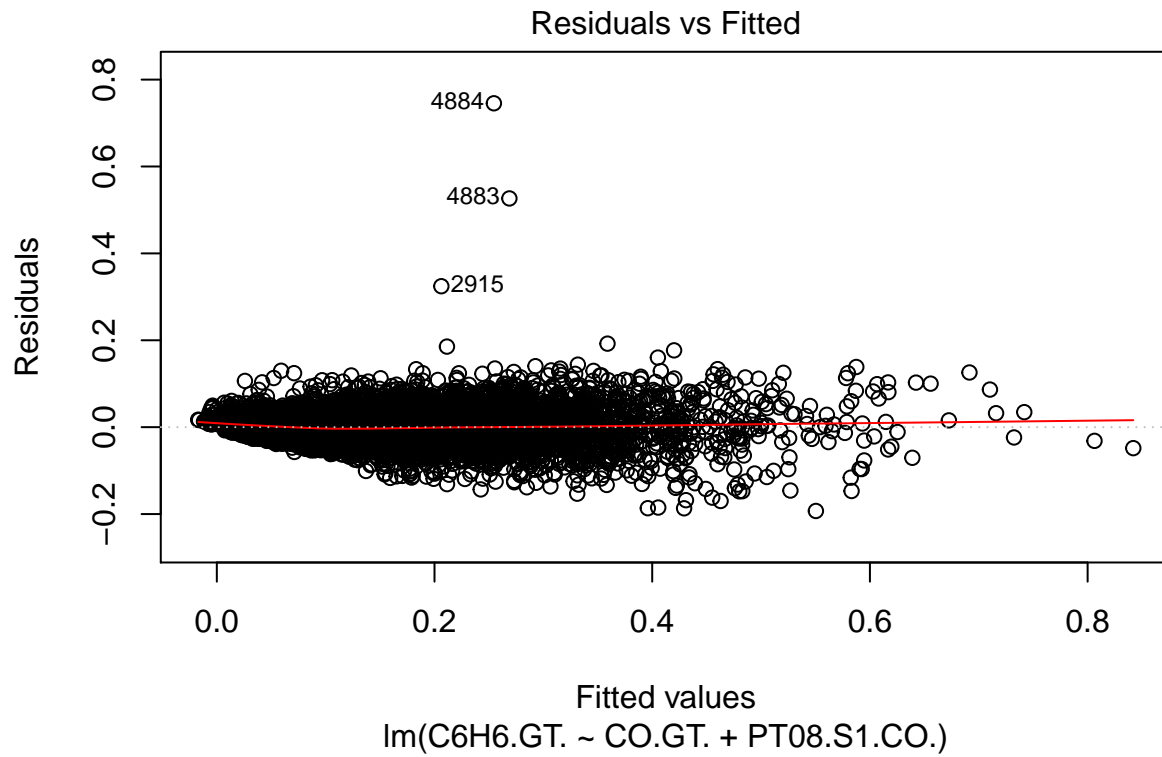
```
## Residual standard error: 0.04048 on 6938 degrees of freedom
## Multiple R-squared:  0.8815, Adjusted R-squared:  0.8814
## F-statistic: 2.58e+04 on 2 and 6938 DF,  p-value: < 2.2e-16
```

```
residuals(lm_9) %>% hist(main = "residuals multi regression CO.GT. + PT08.S1.CO predictors")
```

residuals multi regression CO.GT. + PT08.S1.CO predictors



```
plot(lm_9, which = 1)
```



```
# vif < 5:  
#indicates that predictors are not redundant (not providing overlapping data to inform response)  
vif(lm_9)  
  
##      CO.GT. PT08.S1.CO.  
## 4.331877 4.331877
```