Assumptions & Diagnostics

Utrecht University Winter School: Regression in R

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Outline

Assumptions of MLR

The assumptions of the linear model can be stated as follows:

1. The model is linear in the parameters.
   - This is OK: $Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \beta_4 X^2 + \beta_5 X^3 + \varepsilon$
   - This is not: $Y = \beta_0 X^{\beta_1} + \varepsilon$
2. The predictor matrix is *full rank*.
   - $N > P$
   - No X_p can be a linear combination of other predictors.

Assumptions of MLR

3. The predictors are strictly exogenous.
   - The predictors do not correlated with the errors.
   - $\mathrm{Cov}(\hat{Y}, \varepsilon) = 0$
   - $\mathrm{E}[\varepsilon_n] = 0$
4. The errors have constant, finite variance.
   - $\mathrm{Var}(\varepsilon_n) = \sigma^2 < \infty$
5. The errors are uncorrelated.
   - $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0,\ i \neq j$
6. The errors are normally distributed.
   - $\varepsilon \sim \mathrm{N}(0, \sigma^2)$

Assumptions of MLR

The assumption of *spherical errors* combines Assumptions 4 and 5.

$$\mathrm{Var}(\varepsilon) = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ & & \ddots & \\ 0 & 0 & & 0 \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_N$$

We can combine Assumptions 3, 4, 5, and 6 by assuming independent and identically distributed normal errors:

- $\varepsilon \overset{iid}{\sim} \mathrm{N}(0, \sigma^2)$

Consequences of Violating Assumptions

1. If the model is not linear in the parameters, then we're not even working with linear regression.
    - We need to move to entirely different modeling paradigm.
2. If the predictor matrix is not full rank, the model is not estimable.
    - The parameter estimates cannot be uniquely determined from the data.
3. If the predictors are not exogenous, the estimated regression coefficients will be biased.
4. If the errors are not spherical, the standard errors will be biased.
    - The estimated regression coefficients will be unbiased, though.
5. If errors are non-normal, small-sample inferences may be biased.
    - The justification for some tests and procedures used in regression analysis may not hold.

Regression Diagnostics

If some of the assumptions are (grossly) violated, the inferences we make using the model may be wrong.

- We need to check the tenability of our assumptions before leaning too heavily on the model estimates.

These checks are called *regression diagnostics*.

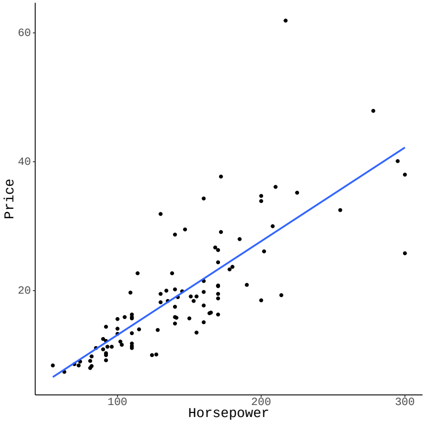
- Graphical visualizations
- Quantitative indices/measures
- Formal statistical tests

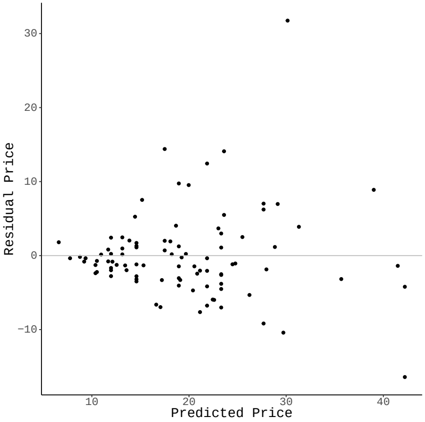
Residual Plots

Plots of residuals vs. predicted values are very useful.

- Here we see clear evidence of heteroscedasticity.

```r
out1 <- lm(Price ~ Horsepower, data = Cars93)
```



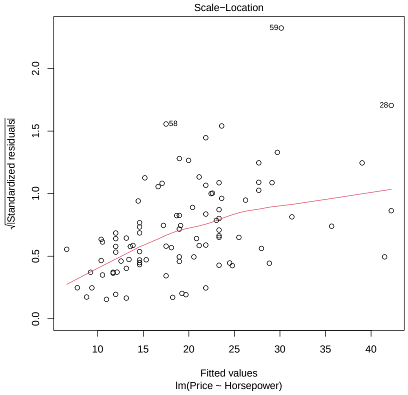


Scale–Location Plots

```r
plot(out1, 3)
```

Scale-location plots also offer an excellent means of detecting non-constant error variance.

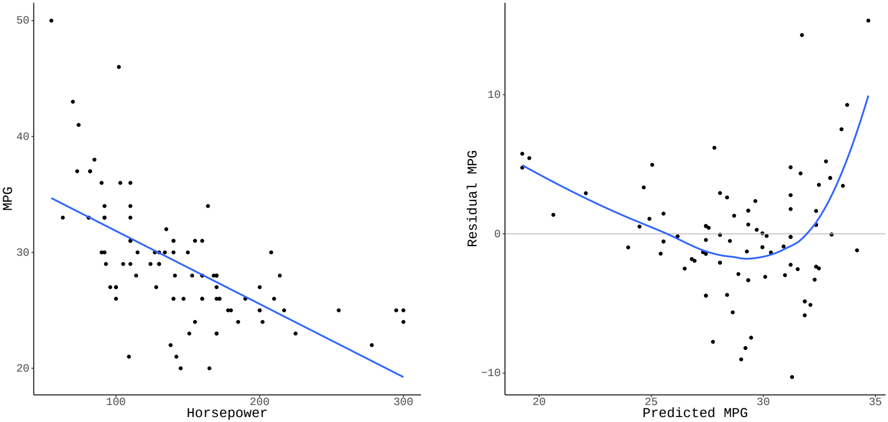
- Plot an approximation of the pointwise residual variance against the fitted values.
- Any trend indicates systematic changes in the residual variance.



Residual Plots

Residual plots can also show violations of the linearity assumption.

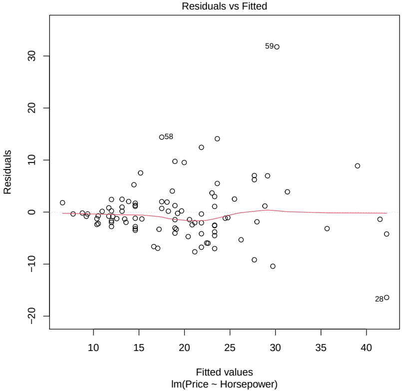
```r
out2 <- lm(MPG.highway ~ Horsepower, data = Cars93)
```



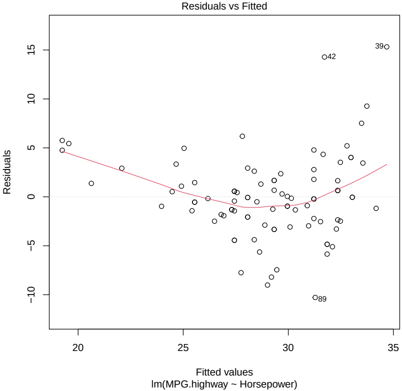
Residual Plots

We can easily create residual plots from a fitted model object.

```r
plot(out1, 1)
```




```r
plot(out2, 1)
```



Partial Residual Plots

In multiple linear regression, ordinary residual plots may not reveal nonlinearity.

- If we do find nonlinearity, ordinary residual plots can't tell us which term is causing the issue.

Partial residual plots show the trend for individual predictors, after controlling for all other variables in the model.

1. First, define the partial residual for the pth predictor.

$$\hat{\varepsilon}_n^{(p)} = \hat{\varepsilon}_n + \hat{\beta}_p X_{np}$$

2. Then, plot the partial residuals, $\hat{\varepsilon}^{(p)}$, against X_p, for all predictors.

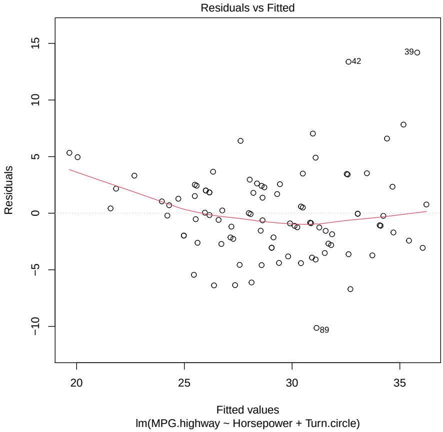
Partial Residual Plots

Let's look at an example. Consider the following model.

```
out3 <- lm(MPG.highway ~ Horsepower + Turn.circle, data = Cars93)
partSummary(out3, -1)

Residuals:
     Min       1Q   Median       3Q      Max 
-10.1346  -2.4247  -0.2107   2.1684  14.1929 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 58.361713   5.339245  10.931  < 2e-16
Horsepower  -0.042480   0.009423  -4.508 1.96e-05
Turn.circle -0.594652   0.153114  -3.884 0.000196

Residual standard error: 3.918 on 90 degrees of freedom
Multiple R-squared:  0.4717,Adjusted R-squared:   0.46 
F-statistic: 40.19 on 2 and 90 DF,  p-value: 3.372e-13
```

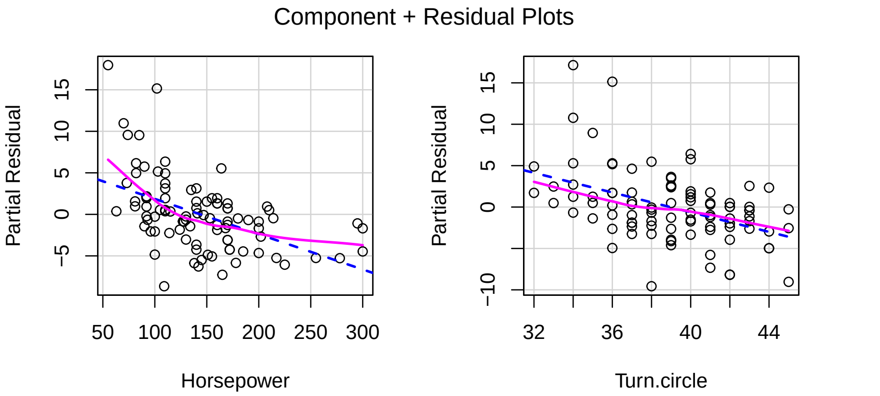
Partial Residual Plots

```r
plot(out3, 1)
```



Partial Residual Plots

```r
crPlots(out3, ylab = "Partial Residual")
```



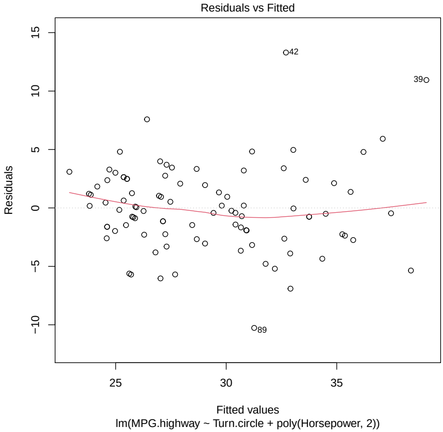
Partial Residual Plots

Let's add the quadratic expansion of Horsepower.

```
out4 <- update(out3, ". ~ . + poly(Horsepower, 2) - Horsepower")
partSummary(out4, -1)

Residuals:
     Min       1Q   Median       3Q      Max
-10.2650  -2.2447  -0.2369   2.3775  13.2971

Coefficients:
                     Estimate Std. Error t value Pr(>|t|)
(Intercept)           43.6770     6.0648   7.202 1.82e-10
Turn.circle           -0.3745     0.1554  -2.411 0.017982
poly(Horsepower, 2)1 -25.1594     4.5537  -5.525 3.24e-07
poly(Horsepower, 2)2  14.6465     3.9757   3.684 0.000394

Residual standard error: 3.67 on 89 degrees of freedom
Multiple R-squared:  0.5416,Adjusted R-squared:  0.5262
F-statistic: 35.06 on 3 and 89 DF,  p-value: 4.729e-15
```

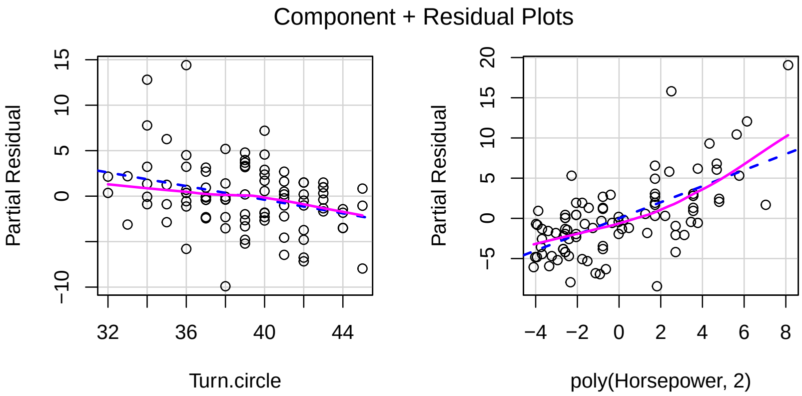
Partial Residual Plots

```r
plot(out4, 1)
```



Partial Residual Plots

```r
crPlots(out4, ylab = "Partial Residual")
```

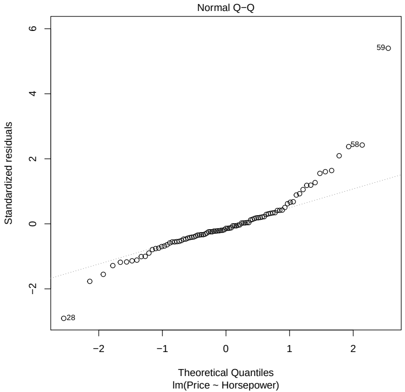


QQ-Plots

```r
plot(out1, 2)
```

A normal Q-Q Plot is one of the best ways to evaluate the normality assumption.

- Plot the quantiles of the residual distribution against the theoretically ideal quantiles.
- We can actually use a Q-Q Plot to compare any two distributions.



Influential Observations

Influential Observations

Influential observations contaminate analyses in two ways:

1. Exert too much influence on the fitted regression model
2. Invalidate estimates/inferences by violating assumptions

There are two distinct types of influential observations:

1. Outliers
    - Observations with extreme outcome values, relative to the other data.
    - Observations with outcome values that fit the model very badly.
2. High-leverage observations
    - Observation with extreme predictor values, relative to other data.

Outliers

Outliers can be identified by scrutinizing the residuals.

- Observations with residuals of large magnitude may be outliers.
- The difficulty arises in quantifying what constitutes a “large” residual.

If the residuals do not have constant variance, then we cannot directly compare them.

- We need to standardize the residuals in some way.

Studentized Residuals

Begin by defining the concept of a *deleted residual*:

$$\hat{\varepsilon}_{(n)} = Y_n - \hat{Y}_{(n)}$$

- $\hat{\varepsilon}_{(n)}$ quantifies the distance of Y_n from the regression line estimated after excluding the nth observation.

If we standardize the deleted residual, $\hat{\varepsilon}_{(n)}$, we get the externally studentized residual:

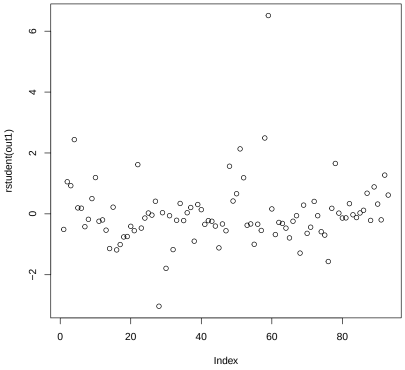
$$t_{(n)} = \frac{\hat{\varepsilon}_{(n)}}{SE_{\hat{\varepsilon}_{(n)}}}$$

Studentized Residual Plots

Index plots of the externally studentized residuals can help spotlight potential outliers.

- Look for observations that clearly "stand out from the crowd."

```r
plot(rstudent(out1))
```



High-Leverage Points

We identify high-leverage observations through their *leverage* values.

- An observation's leverage, h_n, quantifies the extent to which its predictors affect the fitted regression model.
- Observations with X values very far from the mean, $\bar{X}$, affect the fitted model disproportionately.

High-Leverage Points

We identify high-leverage observations through their *leverage* values.

- An observation's leverage, h_n, quantifies the extent to which its predictors affect the fitted regression model.
- Observations with X values very far from the mean, $\bar{X}$, affect the fitted model disproportionately.

In simple linear regression, the nth leverage is given by:

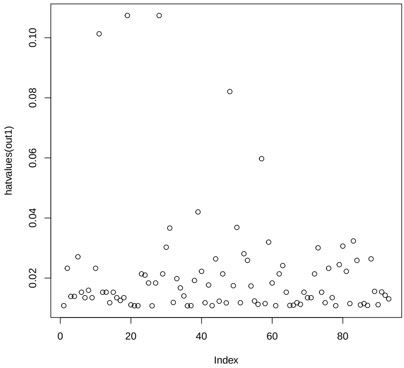
$$h_n = \frac{1}{N} + \frac{\left(X_n - \bar{X}\right)^2}{\sum_{m=1}^{N} \left(X_m - \bar{X}\right)^2}$$

Leverage Plots

```r
plot(hatvalues(out1))
```

Index plots of the leverage values can help spotlight high-leverage points.

- Again, look for observations that clearly "stand out from the crowd."



Outliers & Leverages → Influential Points

Observations with high leverage or large (externally) studentized residuals are not necessarily influential.

- High-leverage observations tend to be more influential than outliers.
- The worst problems arise from observations that are both outliers and have high leverage.

Measures of influence simultaneously consider extremity in both X and Y dimensions.

- Observations with high measures of influence are very likely to cause problems.

Measures of Influence

Measures of influence come in two flavors.

1. Global measures of influence
   - Cook's Distance
2. Coefficient-specific measures of influence
   - DFBETAS

All measures of influence use the same logic as the deleted residual.

- Compare models estimated from the whole sample to models estimated from samples excluding individual observations.

Global Measures of Influence

Each observation gets a Cook's Distance value.

$$\text{Cook's } D_n = \frac{\sum_{n=1}^{N}\left(\hat{Y}_n - \hat{Y}_{(n)}\right)^2}{(P+1)\,\hat{\sigma}^2}$$

$$= (P+1)^{-1} t_n^2 \frac{h_n}{1-h_n}$$

Each regression coefficient (including the intercept) gets a DFBETAS value for each observation.

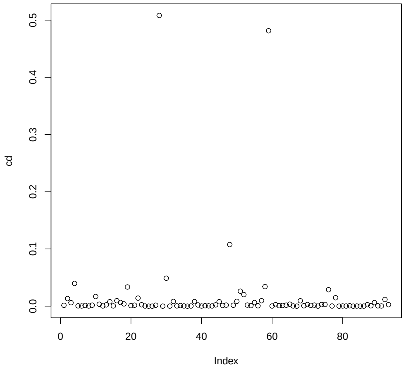
$$\text{DFBETAS}_{np} = \frac{\hat{\beta}_p - \hat{\beta}_{p(n)}}{\text{SE}_{\hat{\beta}_{p(n)}}}$$

Plots of Cook's Distance

```r
cd <- cooks.distance(out1)
plot(cd)
```

Index plots of Cook's distances can help spotlight the influential points.

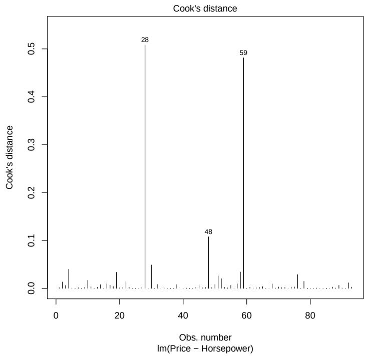
- Look for observations that clearly "stand out from the crowd."



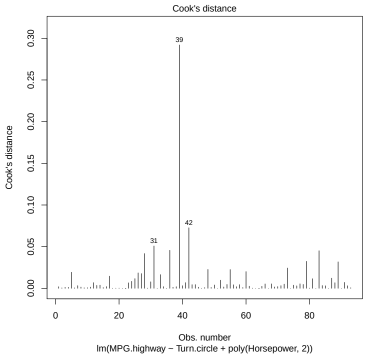
Plots of Cook's Distance

We can create Cook's Distance plots by plotting a fitted model object.

```r
plot(out1, 4)
```

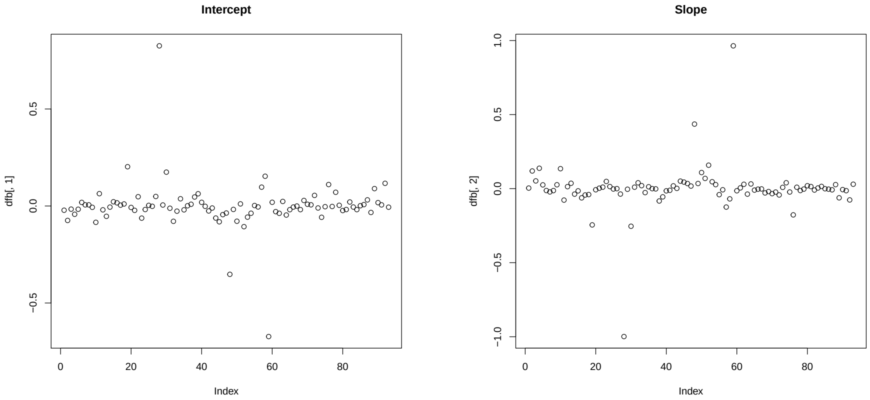



```r
plot(out4, 4)
```



Plots of DFBETAS

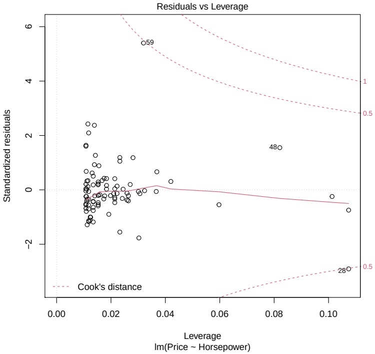
```r
dfb <- dfbetas(out1)
plot(dfb[ , 1], main = "Intercept")
plot(dfb[ , 2], main = "Slope")
```



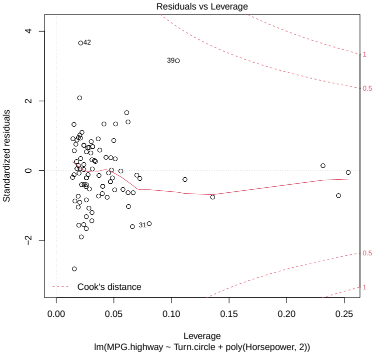
Influence Plots

Plotting studentized residuals against leverages can help identify influential cases.

```r
plot(out1, 5)
```




```r
plot(out4, 5)
```

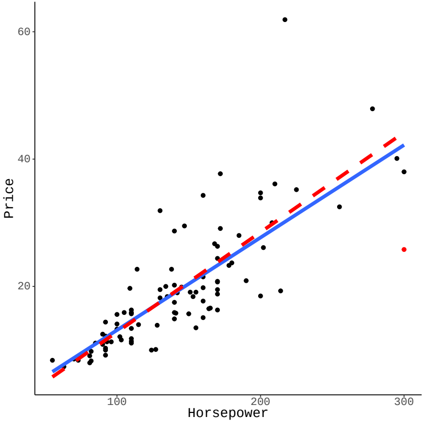


Removing Influential Observations

```r
(maxD <- which.max(cd))

28
28
```

Observation number 28 was the most influential according to Cook's Distance.

- Removing that observation has a small impact on the fitted regression line.
- Influential observations don't only affect the regression line, though.



Removing Influential Observations

```
## Exclude the influential case:
Cars93.2 <- Cars93[-maxD, ]

## Fit model with reduced sample:
out2 <- lm(Price ~ Horsepower, data = Cars93.2)

summary(out1)$coefficients %>% round(6)

             Estimate Std. Error   t value Pr(>|t|)
(Intercept) -1.398769   1.820016 -0.768548 0.444152
Horsepower   0.145371   0.011898 12.218325 0.000000

summary(out2)$coefficients %>% round(6)

             Estimate Std. Error   t value Pr(>|t|)
(Intercept) -2.837646   1.806418 -1.570868 0.119722
Horsepower   0.156750   0.011996 13.066942 0.000000
```

Removing Influential Observations

```
partSummary(out1, 2)

Residuals:
    Min      1Q  Median      3Q     Max
-16.413  -2.792  -0.821   1.803  31.753

partSummary(out2, 2)

Residuals:
     Min       1Q   Median       3Q      Max
-11.4069  -3.0349  -0.5912   1.8530  30.7229
```

Removing Influential Observations

```
summary(out1)[c("sigma", "r.squared", "fstatistic")] %>%
    unlist() %>%
    head(3)

          sigma         r.squared fstatistic.value
       5.976953          0.621287       149.287468

summary(out2)[c("sigma", "r.squared", "fstatistic")] %>%
    unlist() %>%
    head(3)

          sigma         r.squared fstatistic.value
      5.7243112         0.6548351      170.7449721
```

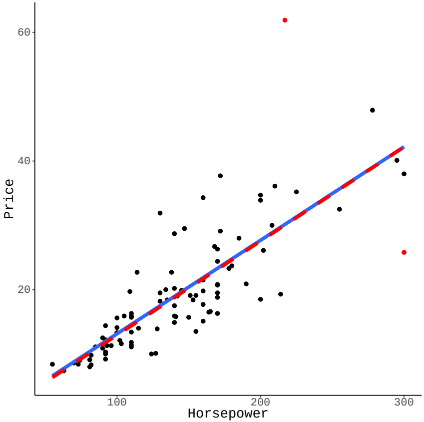
Removing Influential Observations

```
(maxDs <- sort(cd) %>% names() %>% tail(2) %>% as.numeric())
```

```
[1] 59 28
```

If we remove the two most influential observations, 59 and 28, the fitted regression line barely changes at all.

- The influences of these two observations were counteracting one another.
- We're probably still better off, though.



Removing Influential Observations

```r
## Exclude influential cases:
Cars93.2 <- Cars93[-maxDs, ]

## Fit model with reduced sample:
out2.2 <- lm(Price ~ Horsepower, data = Cars93.2)

summary(out1)$coefficients %>% round(6)

              Estimate Std. Error   t value Pr(>|t|)
(Intercept) -1.398769   1.820016 -0.768548 0.444152
Horsepower   0.145371   0.011898 12.218325 0.000000

summary(out2.2)$coefficients %>% round(6)

              Estimate Std. Error   t value Pr(>|t|)
(Intercept) -1.695315   1.494767 -1.134166  0.25977
Horsepower   0.146277   0.009986 14.648807  0.00000
```

Removing Influential Observations

```
partSummary(out1, 2)

Residuals:
    Min      1Q  Median      3Q     Max
-16.413  -2.792  -0.821   1.803  31.753

partSummary(out2.2, 2)

Residuals:
     Min       1Q   Median       3Q      Max
-10.3079  -2.5786  -0.6084   1.9775  14.5793
```

Removing Influential Observations

```
summary(out1)[c("sigma", "r.squared", "fstatistic")] %>%
    unlist() %>%
    head(3)

          sigma          r.squared fstatistic.value
       5.976953           0.621287       149.287468

summary(out2.2)[c("sigma", "r.squared", "fstatistic")] %>%
    unlist() %>%
    head(3)

          sigma          r.squared fstatistic.value
      4.7053314          0.7068391      214.5875491
```