Wednesday, February 18

Mathematical (statistical) models make *assumptions*, and results (statistical inferences) based on the models are derived using those assumptions.

Example: Assume that an object is a *cone*. It can be shown (with a little calculus) that

$$\mathrm{V} = \pi r^2 h/3 \quad \text{and} \quad \mathrm{A} = \pi r \left(r + \sqrt{r^2 + h^2} \right),$$

based on the assumption that *the object is a cone.*

"*All models are wrong but some are useful.*" — George E. P. Box

Implicit Assumptions of Linear and Nonlinear Regression

Discussions of assumptions are based on an alternative representation of a regression model. A linear model can be written as

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i,$$

and a nonlinear model can be written as

$$Y_i = f(x_{i1}, x_{i2}, \ldots, x_{ik}) + \epsilon_i,$$

where the linear model with

$$f(x_{i1}, x_{i2}, \ldots, x_{ik}) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik}$$

is a special case.

There are four implicit assumptions about ϵ_i that go into the derivation of routine/default methods for making inferences concerning the model.

1. $E(\epsilon_i) = 0$ for all i.
2. $Var(\epsilon_i) = \sigma^2$ for all i.
3. $Cov(\epsilon_i, \epsilon_{i'}) = 0$ for all $i \neq i'$.
4. Each ϵ_i has a normal distribution.

How should we approach each assumption?

1. How do we *define* each assumption?
2. What are the *consequences* if the assumption is (very) wrong?
3. How do we *detect* if the assumption is (very) wrong?
4. What is/are the *solution(s)* if the assumption is (very) wrong?

Assumption 1: Zero Expectations of Errors

Definition: The assumption $E(\epsilon_i) = 0$ implies that $E(Y_i)$ depends on the explanatory variables in the way assumed by the model. That is, if we have the *assumed* model

$$E(Y_i) = f(x_{i1}, x_{i2}, \ldots, x_{ik})$$

then

$$E(\epsilon_i) = 0 \Rightarrow E(Y_i) = f(x_{i1}, x_{i2}, \dots, x_{ik}).$$

For the model to be a correct representation of the relationship between $E(Y_i)$ and $x_{i1}, x_{i2}, \dots, x_{ik}$ we require that $E(\epsilon_i) = 0$ for all $i = 1, 2, \dots, n$.

Consequences: Estimates of parameters or some functions thereof (e.g., linear combinations) may be *biased*.

Detection: *Residuals* are statistics that are frequently used to *empirically* investigate assumption violations. There are several types of residuals.

1. Raw residuals. These are simply *estimates* of ϵ_i. In a linear model, for example, the error is

$$\epsilon_i = Y_i - (\beta_0 + \beta_1 x_{i1} + \cdots + \beta_k x_{ik}),$$

   by definition, so a simple estimator of ϵ_i is the *residual*

$$e_i = Y_i - \hat{Y}_i,$$

   where

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \cdots + \hat{\beta}_k x_{ik}.$$

   We can define the raw residual in a similar way for a nonlinear model.

2. Standardized residuals. Defined as

$$z_i = \frac{e_i}{\text{SE}(e_i)}.$$

   If the model assumptions are *correct* then z_i is *approximately* standard normal in distribution so we expect that about 95% of such residuals to satisfy $|z_i| < 2$.

3. Studentized residuals. Defined as

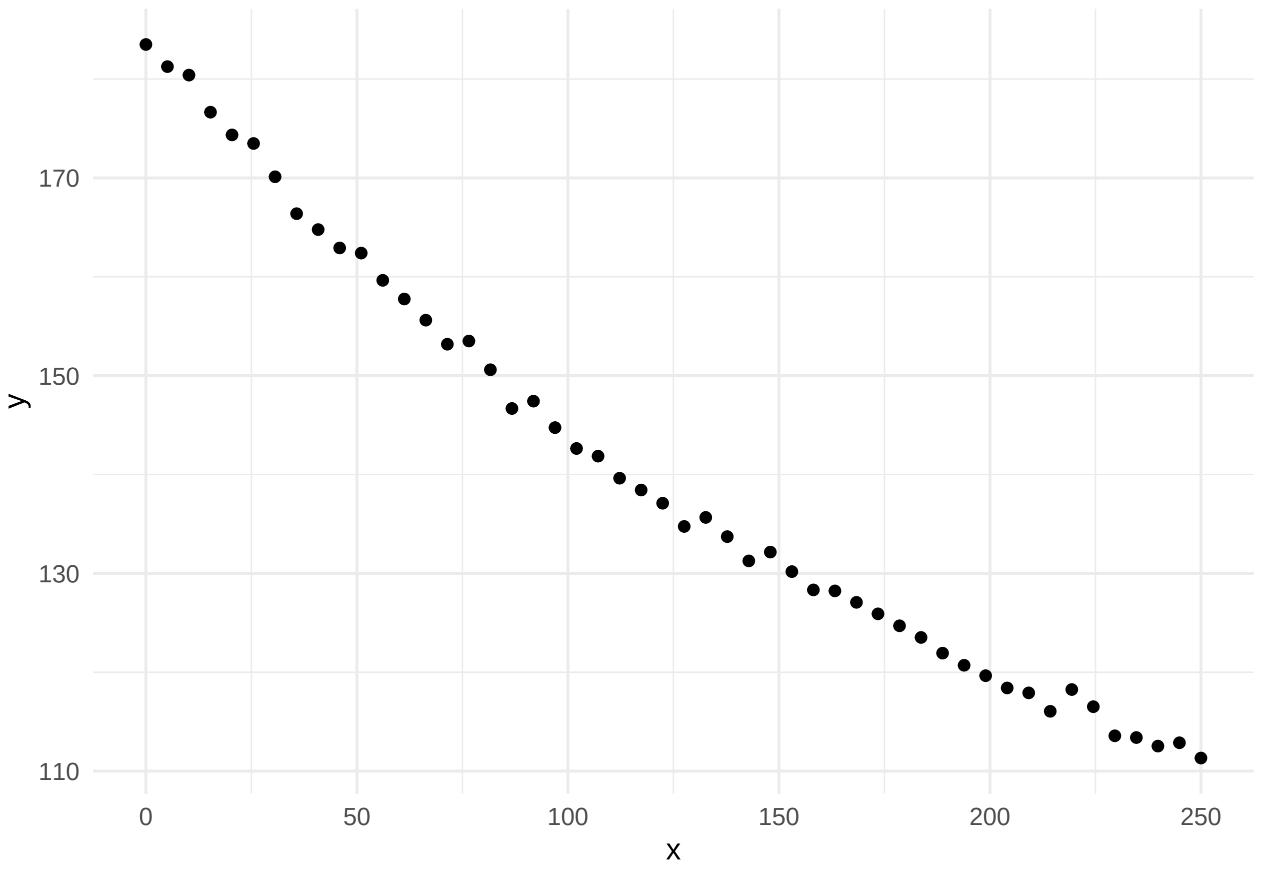
$$t_i = \frac{e_i}{\text{SE}_{(i)}(e_i)},$$

   where $\text{SE}_{(i)}(e_i)$ is the standard error of e_i estimated by *leaving out* that observation. This avoids bias in the standard error in cases where $E(\epsilon_i) \neq 0$. If the model assumptions are met then each t_i has a t distribution with one less degree of freedom than the residual degrees of freedom (i.e., $n - p - 1$ where p is the number of *parameters* in the model). Unless $n - p - 1$ is very small, we expect that about 95% of studentized residuals satisfy $|t_i| < 2$.

What to look for in residuals:

1. Individual observations with exceptional residuals.
2. More residuals than expected overall that are exceptional.
3. Changes in the distribution of residuals when plotting against $\hat{y}_i$.

Example: Consider the following artificial data.

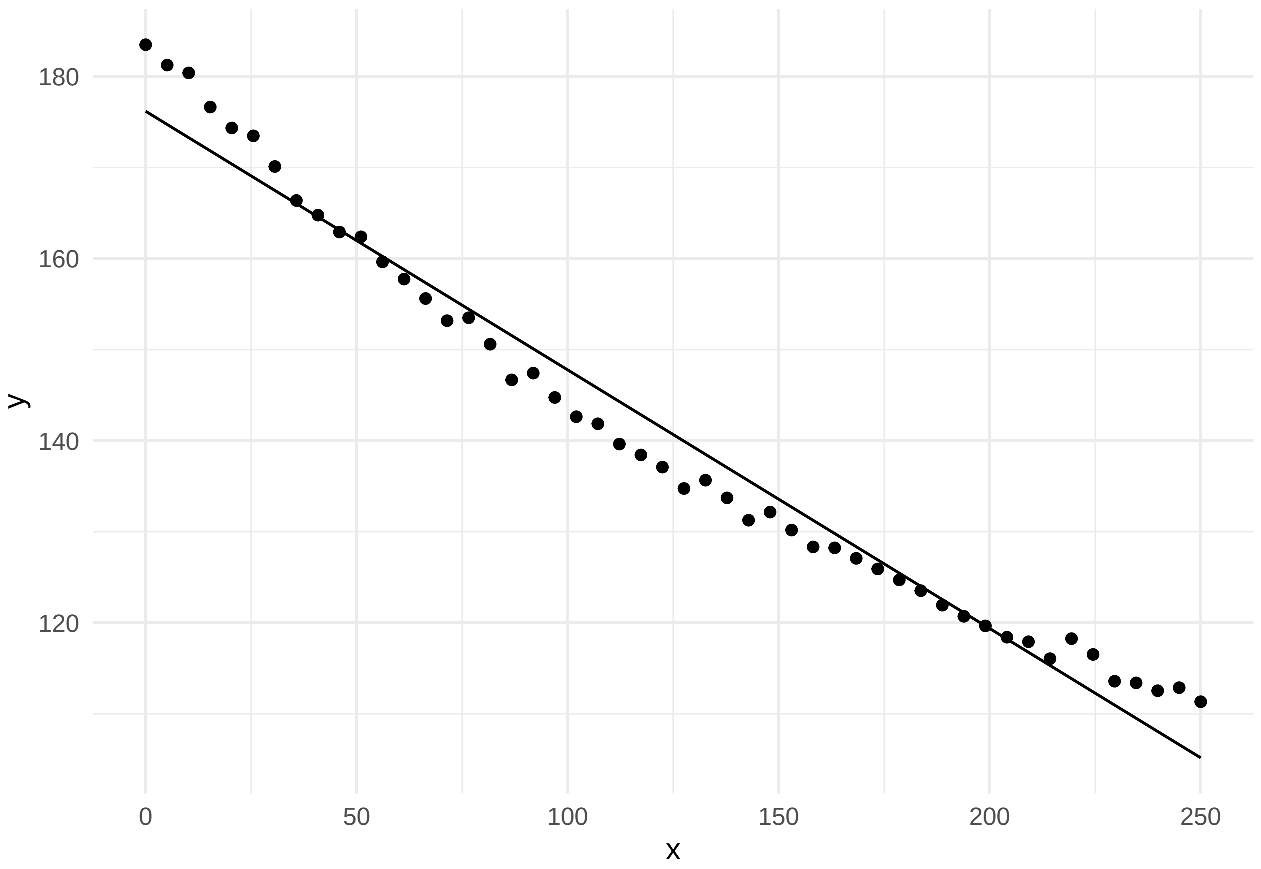


Suppose we tried a linear model.

```
mlinear <- lm(y ~ x, data = fakedata)
fakedata$yhat <- predict(mlinear)   # y-hat values
fakedata$rese <- residuals(mlinear) # raw residuals
fakedata$rest <- rstudent(mlinear)  # studentized residuals
head(fakedata)
```

```
       x     y  yhat  rese  rest
1  0.000 183.5 176.2 7.311 2.198
2  5.102 181.3 174.7 6.525 1.936
3 10.204 180.4 173.3 7.113 2.121
4 15.306 176.6 171.8 4.813 1.396
5 20.408 174.4 170.4 3.964 1.140
6 25.510 173.5 168.9 4.547 1.311
```

```
p <- p + geom_line(aes(y = yhat), data = fakedata)
plot(p)
```



What are the observations with "exceptionally large" residuals?

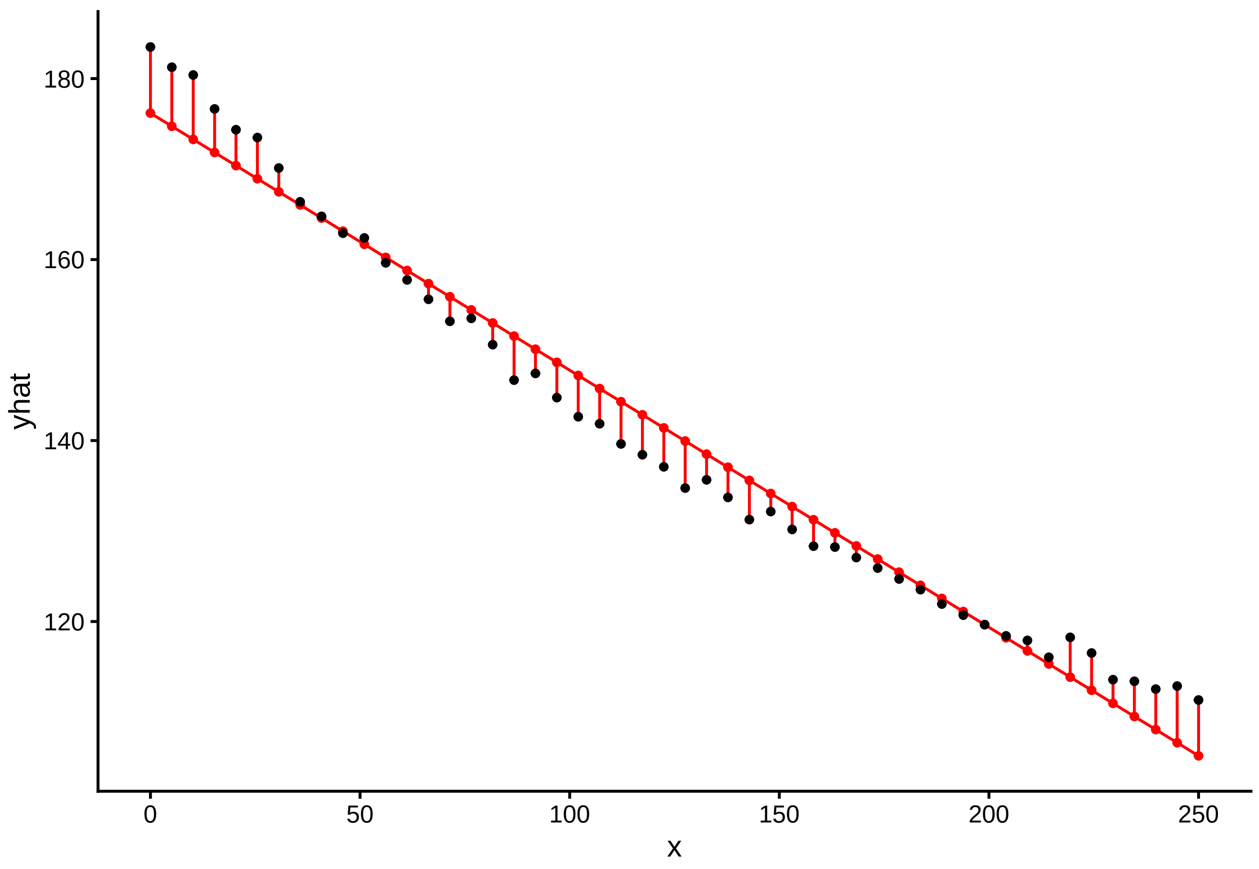
```
subset(fakedata, abs(rest) > 2)
```

```
     x     y  yhat  rese  rest
1  0.0 183.5 176.2 7.311 2.198
3 10.2 180.4 173.3 7.113 2.121
```

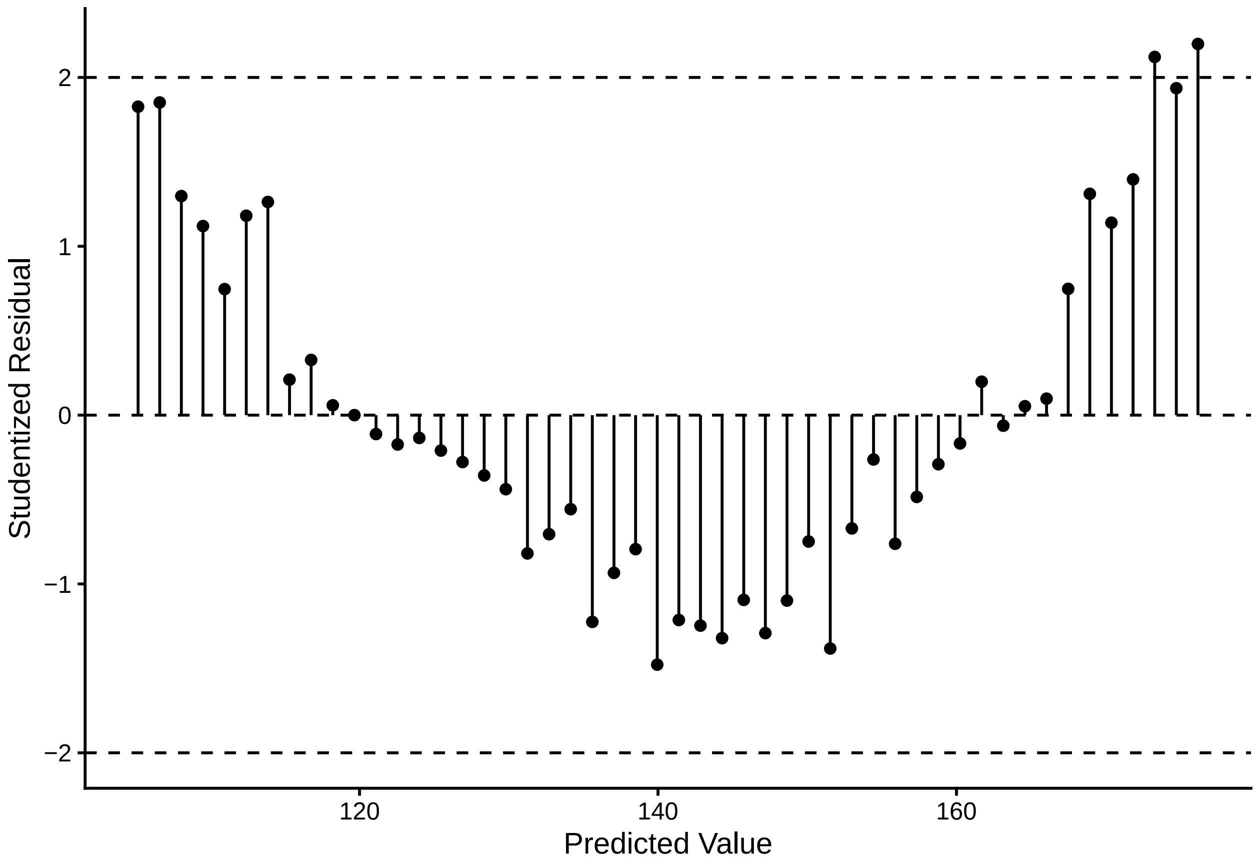
```
library(dplyr)
fakedata %>% filter(abs(rest) > 2)
```

```
     x     y  yhat  rese  rest
1  0.0 183.5 176.2 7.311 2.198
2 10.2 180.4 173.3 7.113 2.121
```

Are there any patterns?



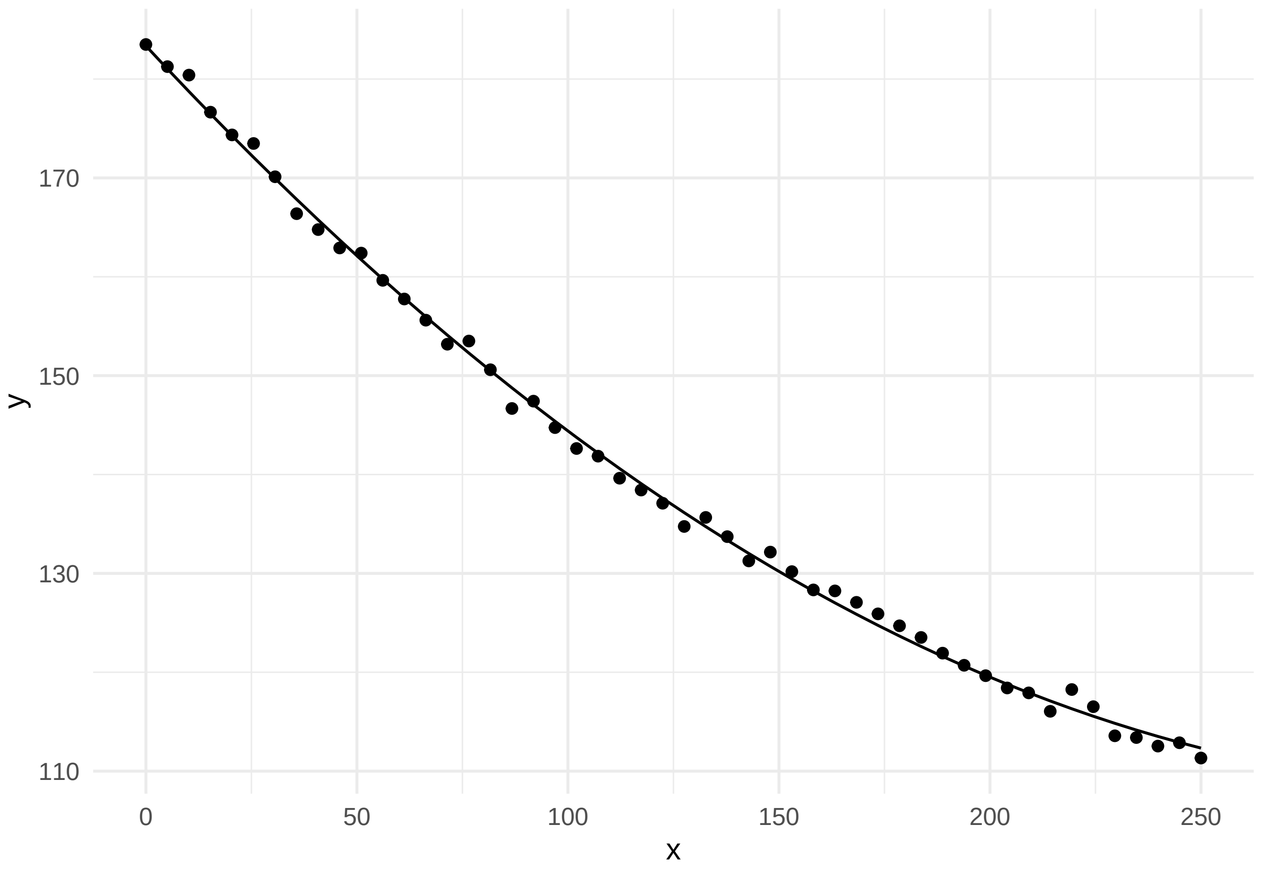
```r
p <- ggplot(fakedata, aes(x = yhat, y = rest))
p <- p + geom_segment(aes(x = yhat, xend = yhat, y = 0, yend = rest))
p <- p + geom_point() + theme_classic()
p <- p + labs(x = "Predicted Value", y = "Studentized Residual")
p <- p + geom_hline(yintercept = c(-2, 0, 2), linetype = 2)
plot(p)
```



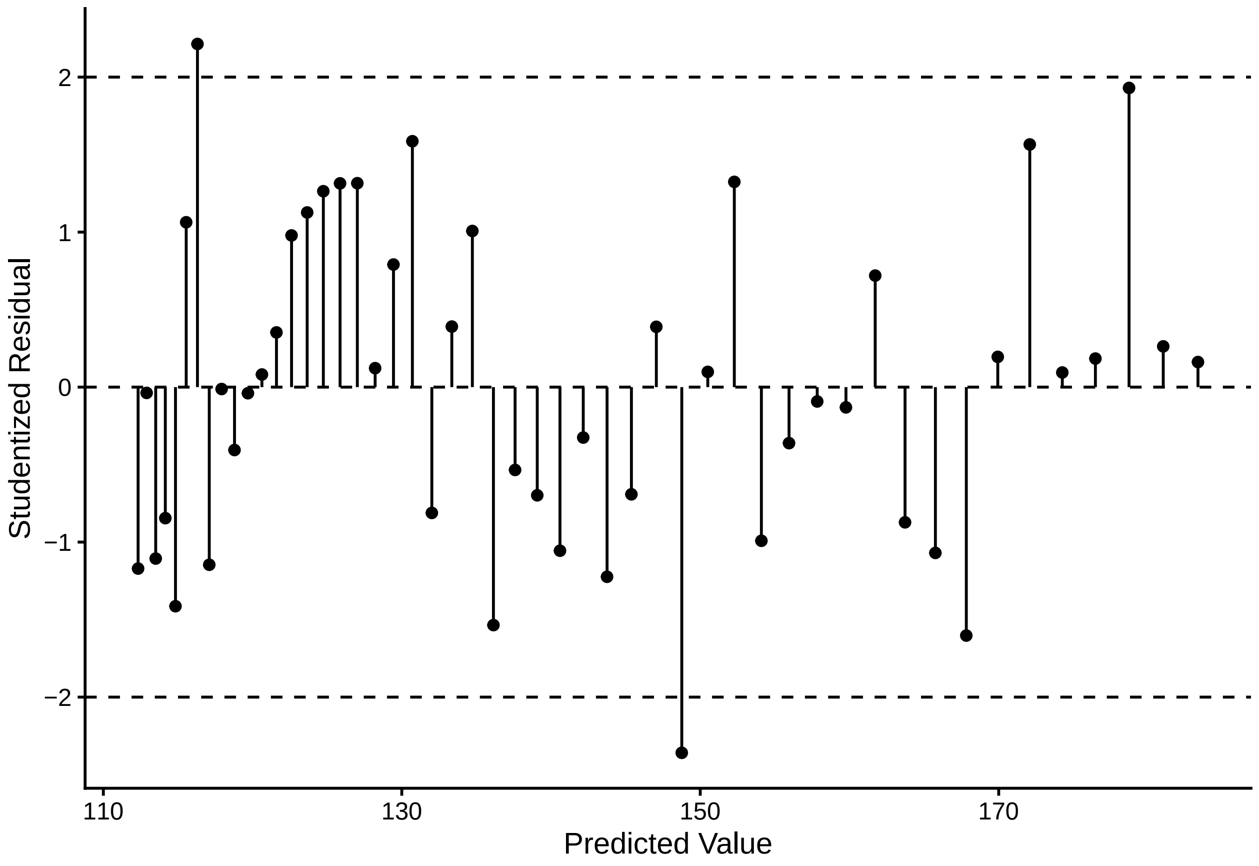
Let's try the polynomial model $E(Y_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$.

```
mpoly <- lm(y ~ poly(x, degree = 2), data = fakedata)
fakedata$yhat <- predict(mpoly)
fakedata$rest <- rstudent(mpoly)

p <- ggplot(fakedata, aes(x = x, y = y)) + theme_minimal()
p <- p + geom_point() + geom_line(aes(y = yhat))
plot(p)
```



```r
p <- ggplot(fakedata, aes(x = yhat, y = rest)) +
  geom_segment(aes(x = yhat, xend = yhat, y = 0, yend = rest)) +
  geom_point() + theme_classic() +
  labs(x = "Predicted Value", y = "Studentized Residual") +
  geom_hline(yintercept = c(-2, 0, 2), linetype = 2)
plot(p)
```



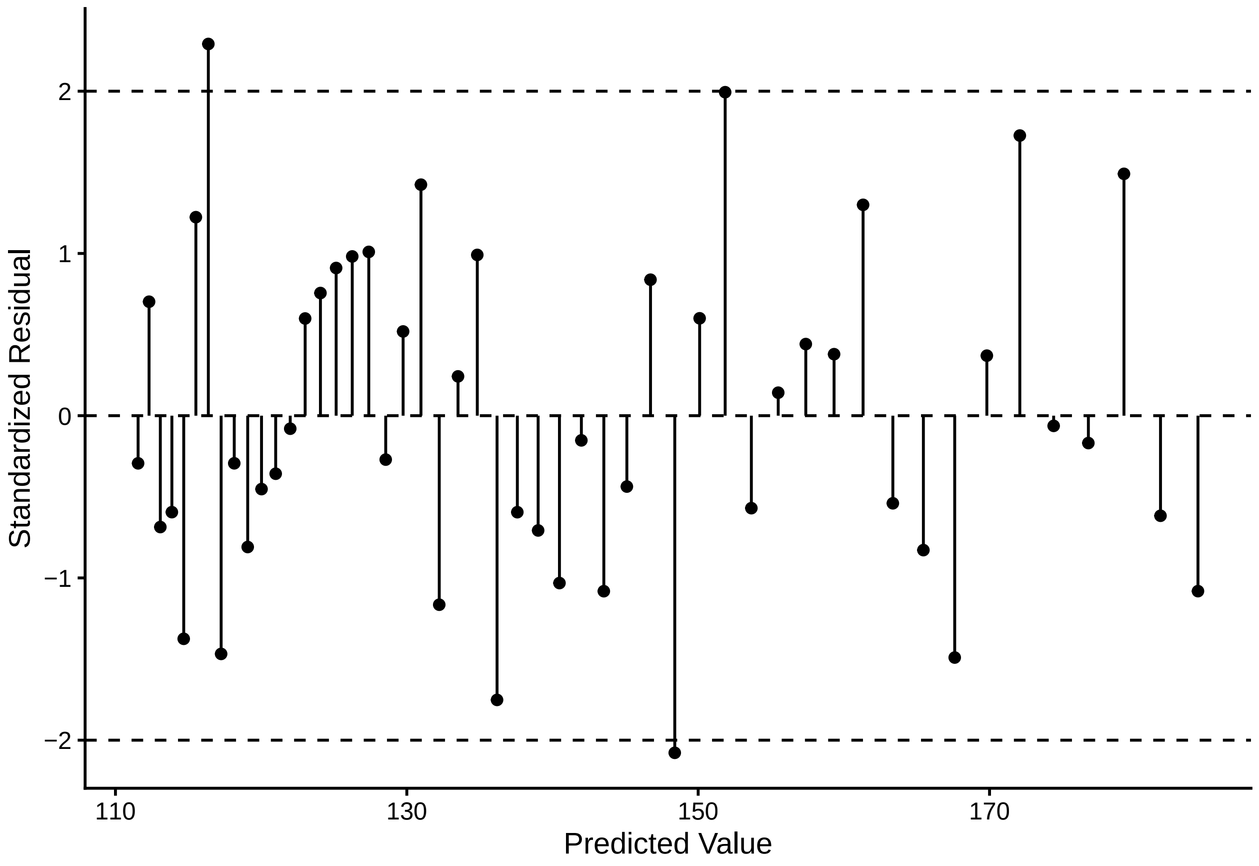
The "correct" model is the nonlinear model

$$E(Y_i) = \alpha + (\delta - \alpha)2^{-x_i/\gamma}.$$

```
mnlin <- nls(y ~ alpha + (delta - alpha) * 2^(-x / gamma),
  data = fakedata, start = list(alpha = 80, delta = 180, gamma = 140))
library(trtools) # for the nlsint function
d <- nlsint(mnlin, residuals = TRUE)
head(d)
```

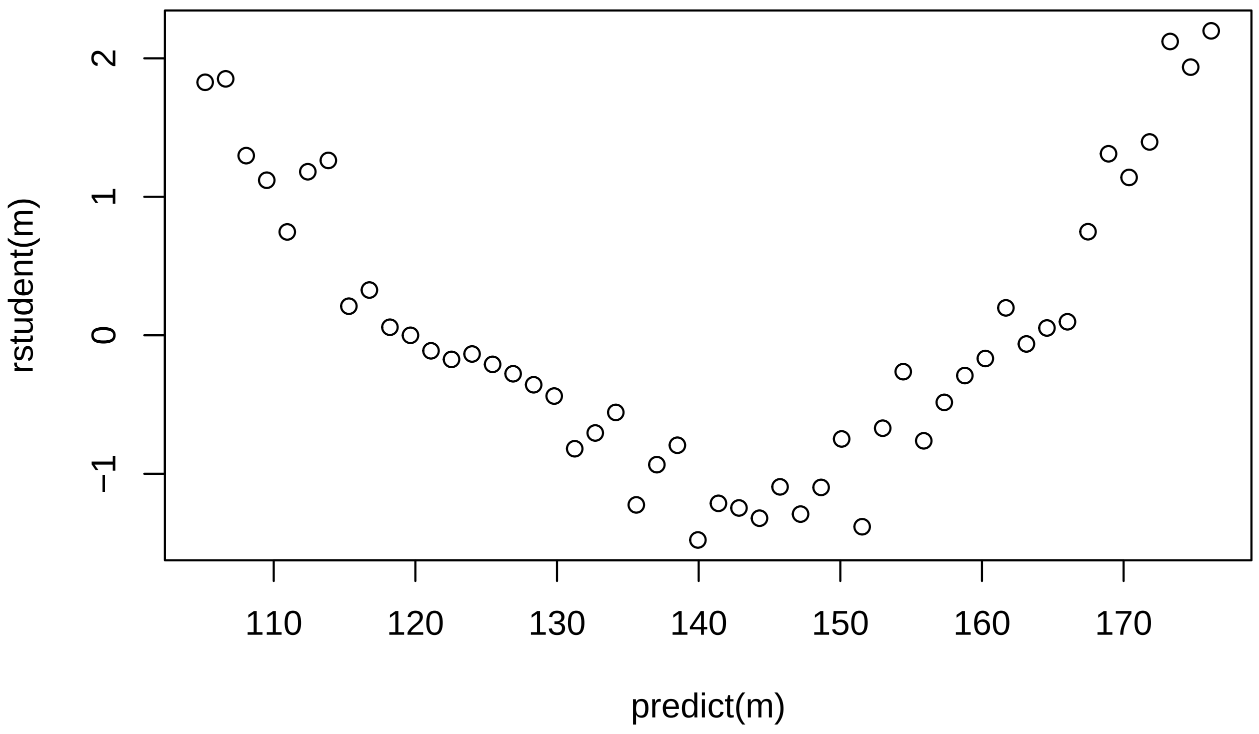
```
    fit     se   lwr   upr     hat      res
1 184.3 0.3894 183.5 185.1 0.21231 -1.08147
2 181.7 0.3481 181.0 182.4 0.16966 -0.61684
3 179.2 0.3112 178.6 179.9 0.13564  1.49073
4 176.8 0.2788 176.2 177.3 0.10888 -0.16877
5 174.4 0.2510 173.9 174.9 0.08820 -0.06274
6 172.1 0.2276 171.6 172.5 0.07256  1.72687
```

```
p <- ggplot(d, aes(x = fit, y = res)) +
  geom_segment(aes(x = fit, xend = fit, y = 0, yend = res)) +
  geom_point() + theme_classic() +
  labs(x = "Predicted Value", y = "Standardized Residual") +
  geom_hline(yintercept = c(-2, 0, 2), linetype = 2)
plot(p)
```

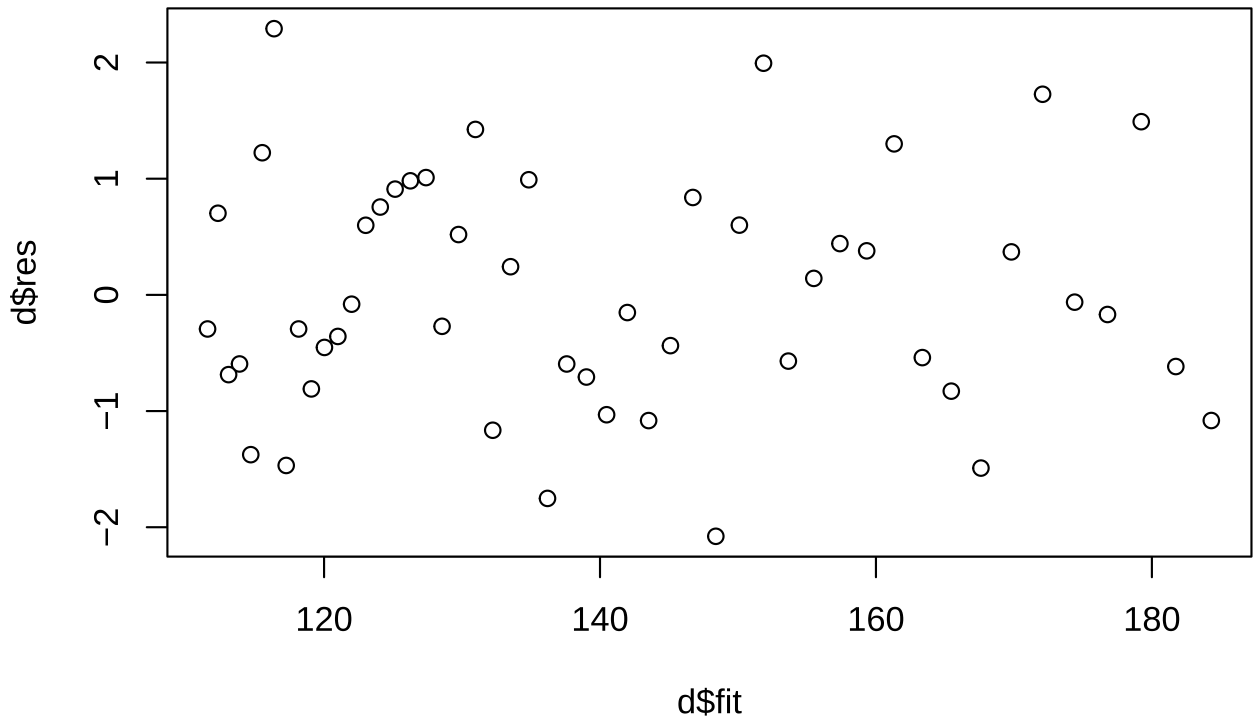


Note that since we are usually not interested in created publication quality residual plots, we can do some quick-and-dirty plots with simpler (but uglier) graphics.

```
# when using lm
m <- lm(y ~ x, data = fakedata)
plot(predict(m), rstudent(m))
```



```
# when using nls
mnlin <- nls(y ~ alpha + (delta - alpha) * 2^(-x / gamma),
  data = fakedata, start = list(alpha = 80, delta = 180, gamma = 140))
d <- nlsint(mnlin, residuals = TRUE) # nlsint is from trtools package
plot(d$fit, d$res)
```

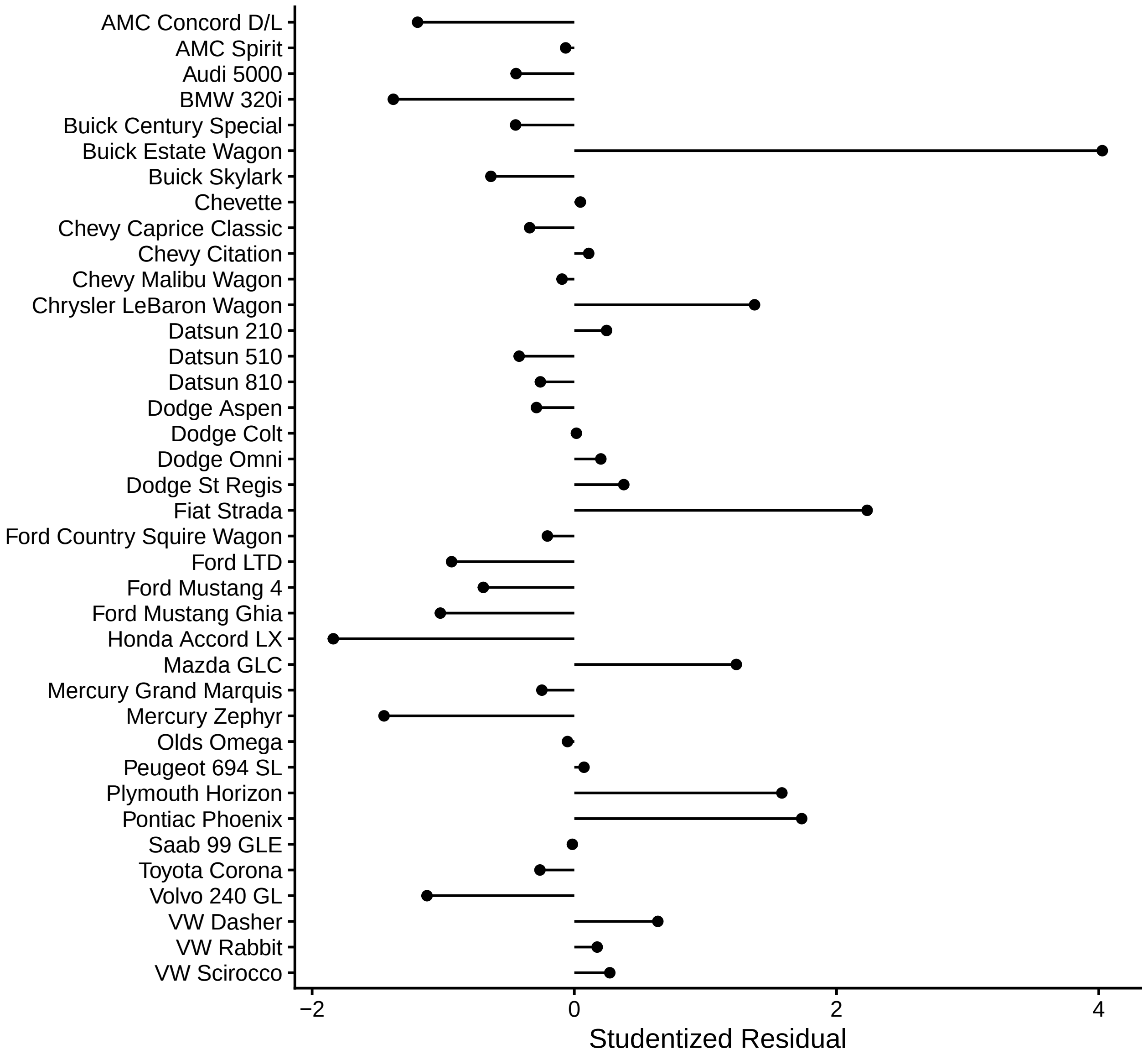


Example: Consider a model where the expected MPG of cars is assumed to be a linear function of weight and rear axle ratio.

```r
library(dplyr)
cars <- read.csv("https://raw.githubusercontent.com/trobinj/stat516/refs/heads/gh-pages/cars.csv")
cars <- cars |> select(car, mpg, weight, hp, ratio)
m <- lm(mpg ~ weight + hp + ratio, data = cars)
cars$yhat <- predict(m)
cars$rest <- rstudent(m)
subset(cars, abs(rest) > 2)
```

```
                  car  mpg weight  hp ratio  yhat  rest
1  Buick Estate Wagon 16.9   4.36 155  2.73 10.31 4.027
34        Fiat Strada 37.3   2.13  69  3.10 32.93 2.233
```

```r
p <- ggplot(cars, aes(x = rest, y = car)) + geom_point() +
  theme_classic() + scale_y_discrete(limits = rev) +
  geom_segment(aes(x = 0, xend = rest, y = car, yend = car)) +
  labs(x = "Studentized Residual", y = NULL)
plot(p)
```



What is up with the Buick Estate Wagon?

Solutions: Modify the model. Drop offending observation(s) if and only if you can justify restricting the scope of the model.

Assumption 2: Equality of Error Variances

Definition: In the regression model

$$Y_i = f(x_{i1}, x_{i2}, \dots, x_{ik}) + \epsilon_i,$$

we assume $\text{Var}(\epsilon_i) = \sigma^2$ which implies $\text{Var}(Y_i) = \sigma^2$. This is called "homoscedasticty" or sometimes "homogeneity of variance" in the context of linear models for designed experiments. A more complete description of the assumed model is

$$E(Y_i) = f(x_{i1}, x_{i2}, \dots, x_{ik}), \tag{1}$$
$$\text{Var}(Y_i) = \sigma^2. \tag{2}$$

Note that the estimator $\hat{\sigma}^2$, the square of the "residual standard error" reported by `summary`, is computed as

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-p},$$

where p is the number of parameters in the part of the model for $E(Y_i)$ (which is $p = k + 1$ in a linear model with a β_0 term and k explanatory variables).

Consequences: Severe violations of homoscedaticity can result in two problems.

1. Biased standard errors, incorrect p-values, and incorrect confidence/prediction intervals.
2. Inefficient estimation of model parameters (and functions thereof).

Detection: Many common patterns of heteroscedasticity can be found by plotting standardized or studentized residuals against $\hat{y}_i$.

Example: Consider the following data on survival time of terminal cancer patients given a supplement of ascorbate (i.e., vitamin C).

```r
library(Stat2Data)
data(CancerSurvival) # this package requires that we "load" the data
head(CancerSurvival)
```

```
  Survival   Organ
1      124 Stomach
2       42 Stomach
3       25 Stomach
4       45 Stomach
5      412 Stomach
6       51 Stomach
```

For plotting purposes we can order the levels of Organ according to mean survival using `reorder`.

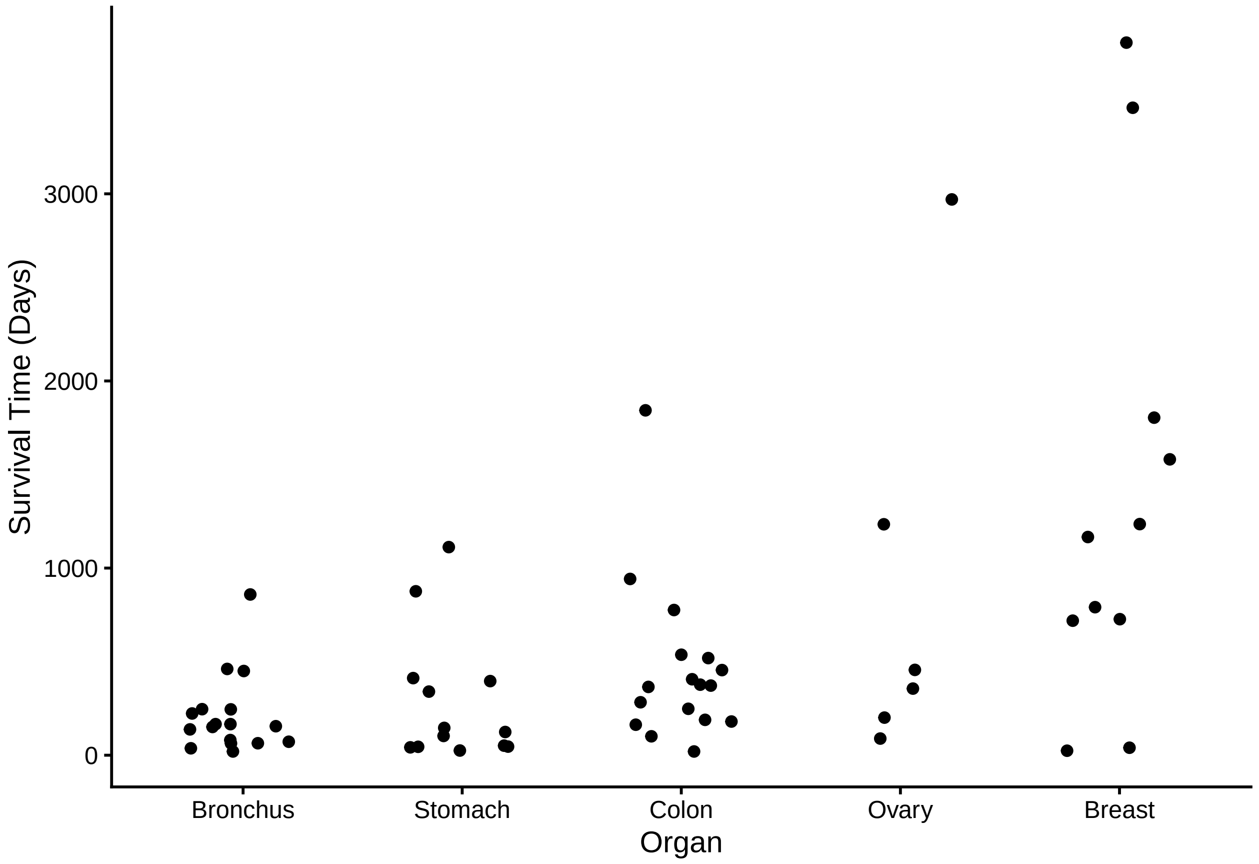
```r
CancerSurvival$Organ <- with(CancerSurvival, reorder(Organ, Survival, mean))
```

The `with` function implies that each variable is "with" the data frame `CancerSurvival`. This is sometimes nicer than having to identify the data frame explicitly as in the following.

```r
CancerSurvival$Organ <- reorder(CancerSurvival$Organ, CancerSurvival$Survival, mean)
```

Here is a plot of the data using `geom_jitter` to space out the points.

```r
p <- ggplot(CancerSurvival, aes(x = Organ, y = Survival)) +
  geom_jitter(height = 0, width = 0.25) +
  labs(y = "Survival Time (Days)") + theme_classic()
plot(p)
```



Here we can see some descriptive statistics.

```r
library(dplyr)
CancerSurvival %>% group_by(Organ) %>%
  summarize(mean = mean(Survival), stdev = sd(Survival), obs = n())
```

```
# A tibble: 5 x 4
  Organ     mean stdev   obs
  <fct>    <dbl> <dbl> <int>
1 Bronchus  212.  210.    17
2 Stomach   286   346.    13
3 Colon     457.  427.    17
4 Ovary     884. 1099.     6
5 Breast   1396. 1239.    11
```

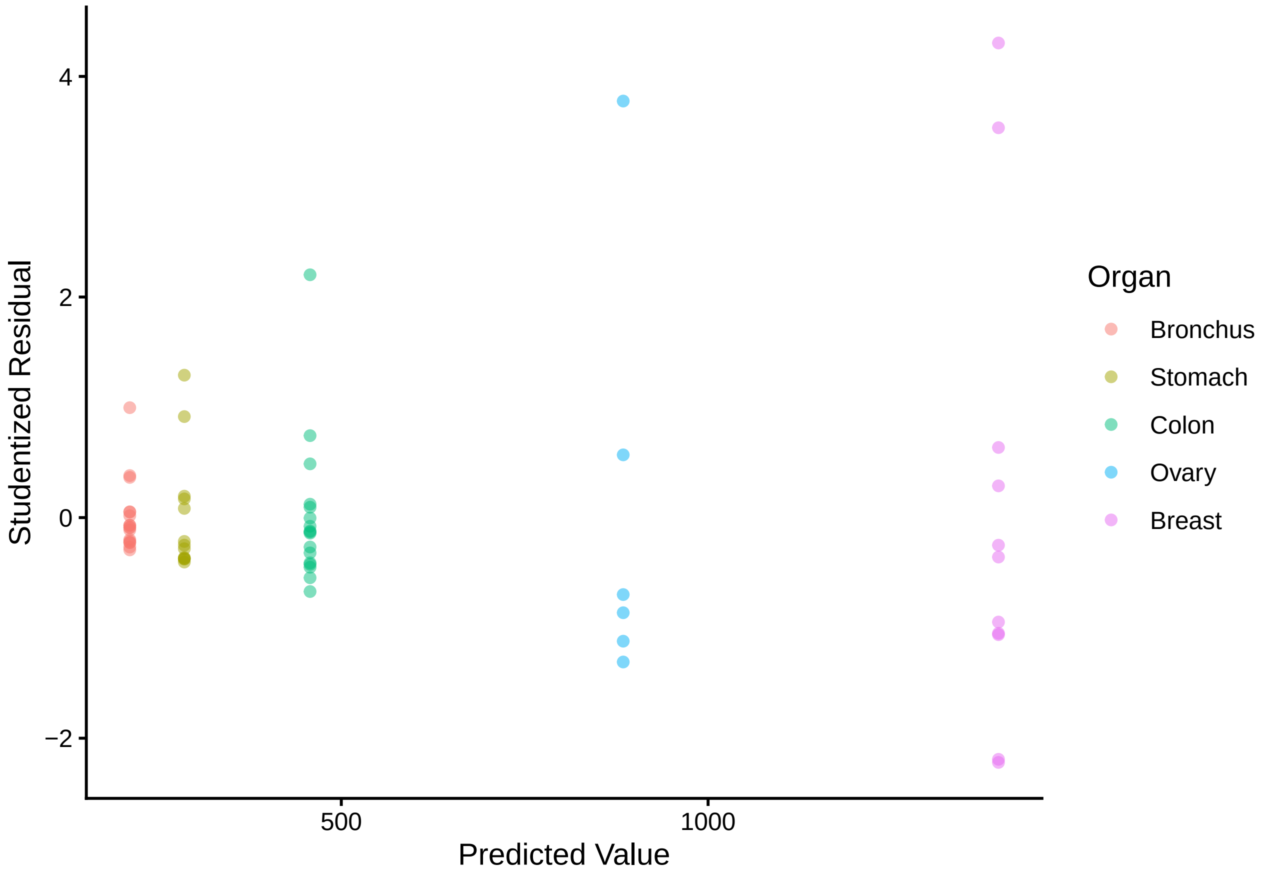
Now consider a linear model that assumes homoscedasticity.

```r
m <- lm(Survival ~ Organ, data = CancerSurvival)
CancerSurvival$yhat <- predict(m)
CancerSurvival$rest <- rstudent(m)
head(CancerSurvival)
```

```
  Survival    Organ yhat    rest
```

```
1      124 Stomach  286 -0.2498
2       42 Stomach  286 -0.3765
3       25 Stomach  286 -0.4029
4       45 Stomach  286 -0.3719
5      412 Stomach  286  0.1943
6       51 Stomach  286 -0.3626
```

```r
p <- ggplot(CancerSurvival, aes(x = yhat, y = rest, color = Organ)) +
  geom_point(alpha = 0.5) + theme_classic() +
  labs(x = "Predicted Value", y = "Studentized Residual")
plot(p)
```



Example: Consider the following data from a study on the effects of fuel reduction on biomass.

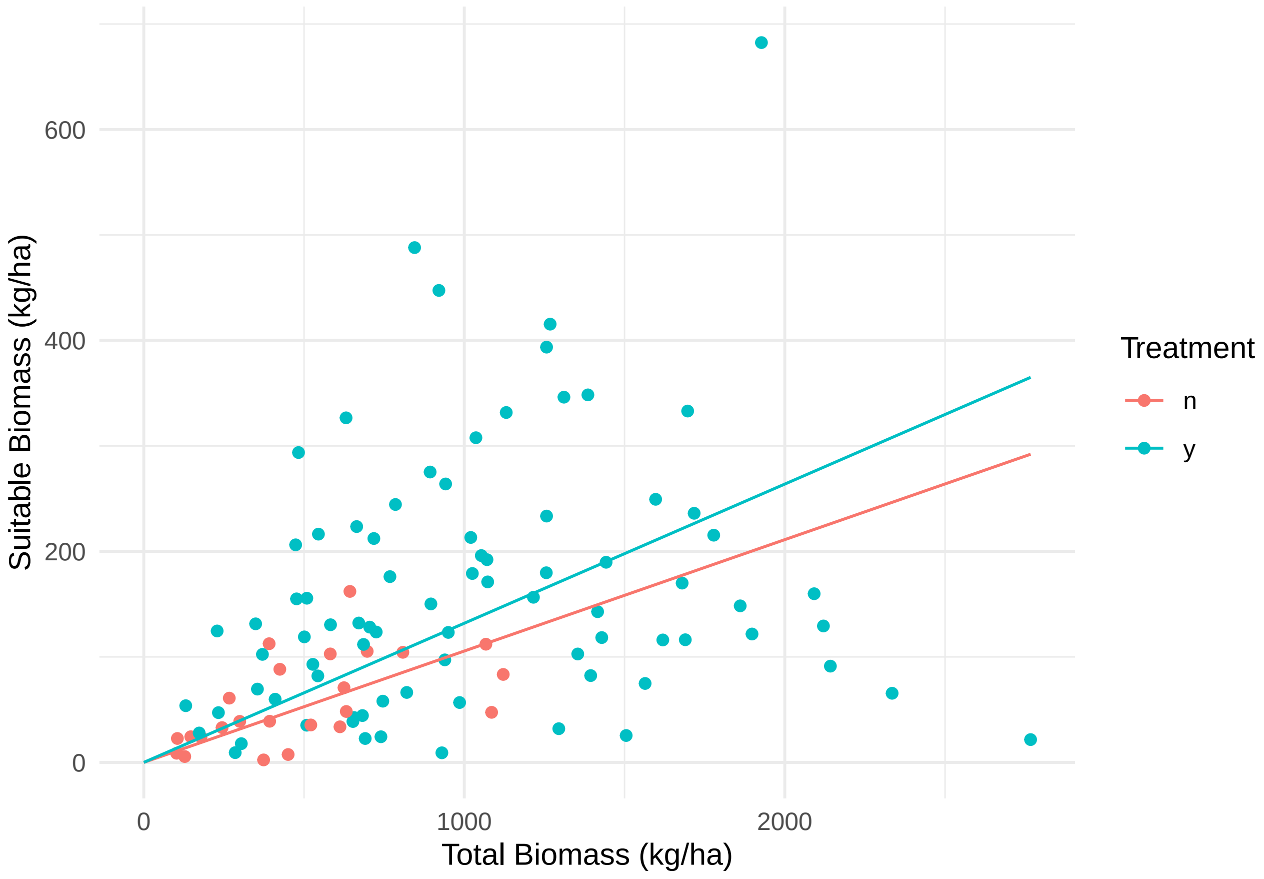
```r
library(trtools) # for biomass data

m <- lm(suitable ~ -1 + treatment:total, data = biomass)
summary(m)$coefficients
```

```
                 Estimate Std. Error t value Pr(>|t|)
treatmentn:total   0.1056    0.04183   2.524 1.31e-02
treatmenty:total   0.1319    0.01121  11.773 7.61e-21
```

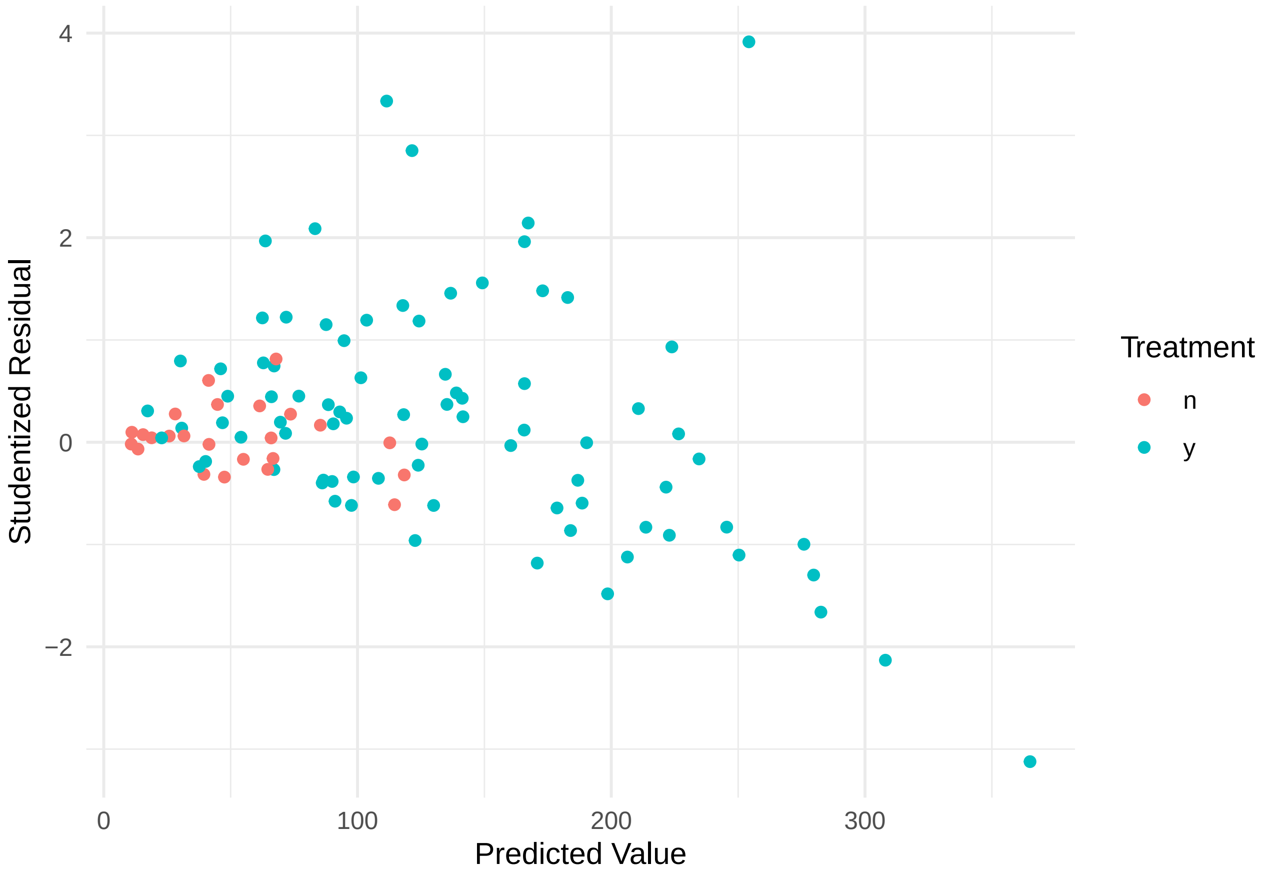
```r
d <- expand.grid(treatment = c("n","y"), total = seq(0, 2767, length = 10))
d$yhat <- predict(m, newdata = d)

p <- ggplot(biomass, aes(x = total, y = suitable, color = treatment)) +
  geom_point() + geom_line(aes(y = yhat), data = d) + theme_minimal() +
  labs(x = "Total Biomass (kg/ha)", y = "Suitable Biomass (kg/ha)",
    color = "Treatment")
plot(p)
```



```
biomass$yhat <- predict(m)
biomass$rest <- rstudent(m)

p <- ggplot(biomass, aes(x = yhat, y = rest, color = treatment)) +
  geom_point() + theme_minimal() +
  labs(x = "Predicted Value", y = "Studentized Residual",
    color = "Treatment")
plot(p)
```



Solutions: There are several possible solutions.

1. Response variable transformation.
2. Weighted least squares.
3. Robust standard error estimators.
4. Models that do not assume constant variance.

We will discuss each of these in turn soon.