

Monday, Feb 12

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

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

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

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

where the linear model with

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

is a special case.

There are four implicit assumptions about  $\epsilon_i$  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  $\epsilon_i$  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

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

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  $\epsilon_i$ . In a linear model, for example, the error is

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

by definition, so a simple estimator of  $\epsilon_i$  is the *residual*

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

where

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

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

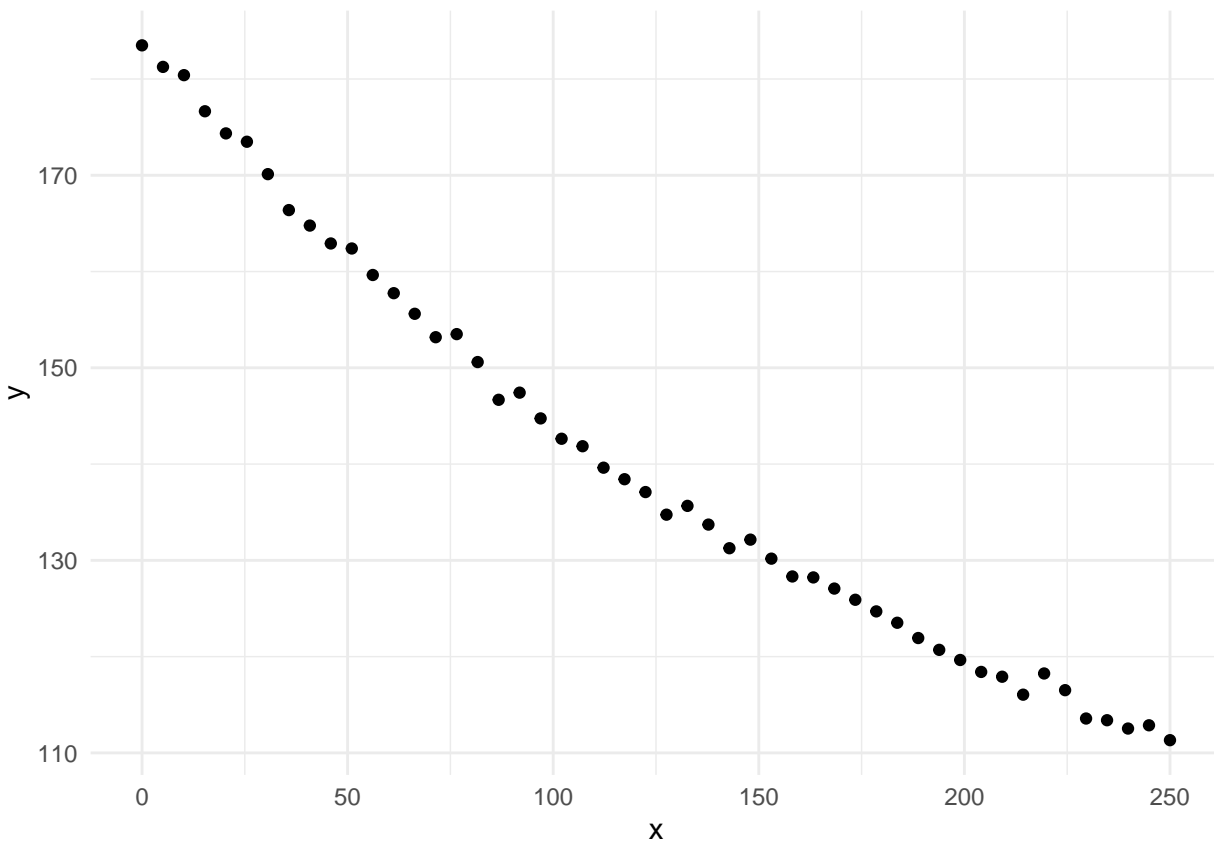
$$t_i = \frac{e_i}{\text{SE}_{(i)}(e_i)},$$

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.

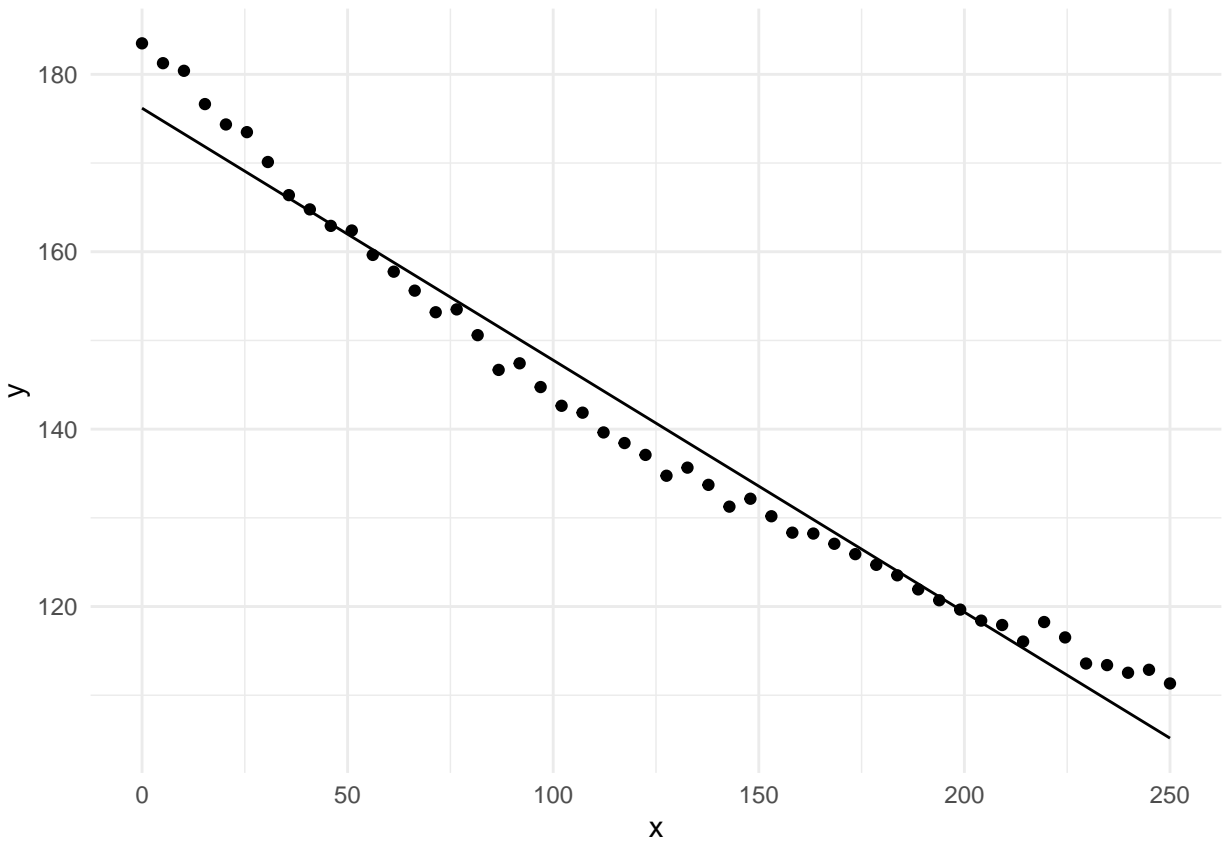


Suppose we tried a linear model.

```
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?

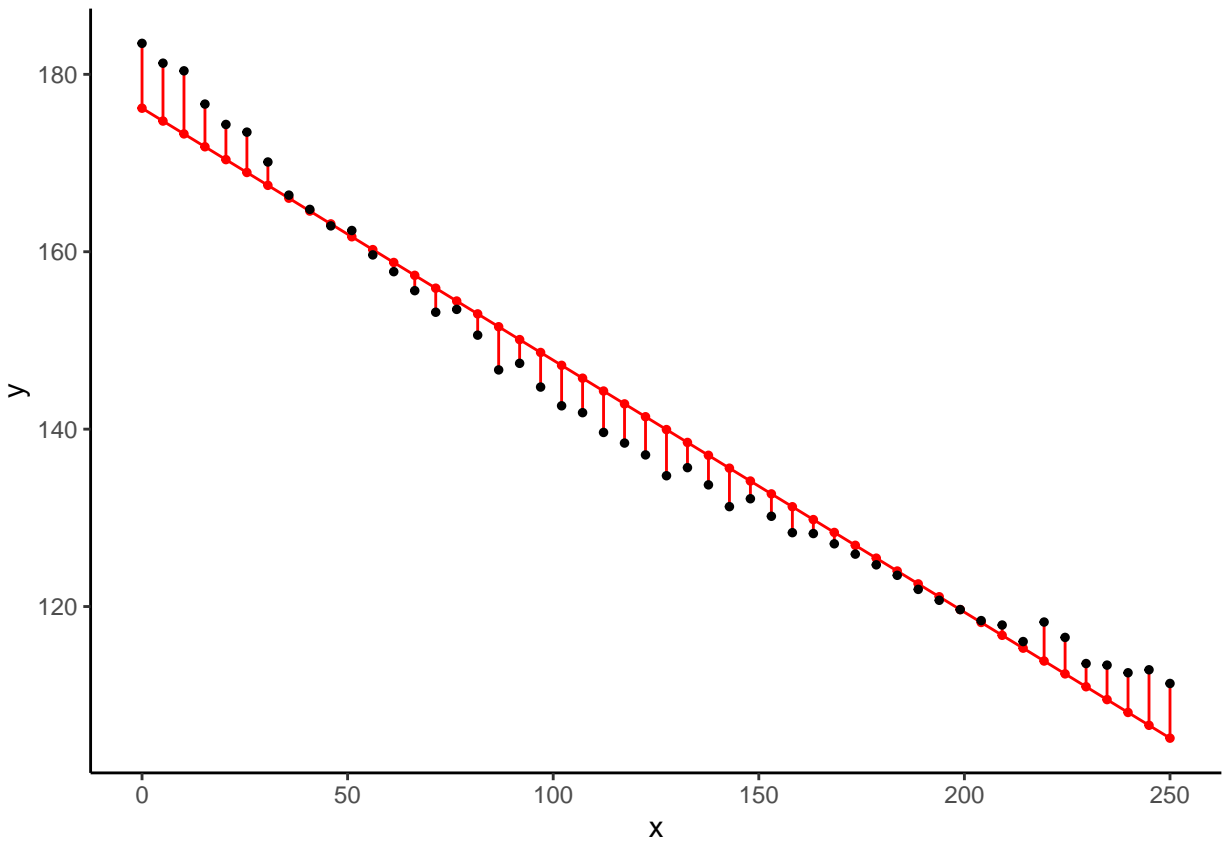
```
subset(fakedata, abs(rest) > 2)
```

	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

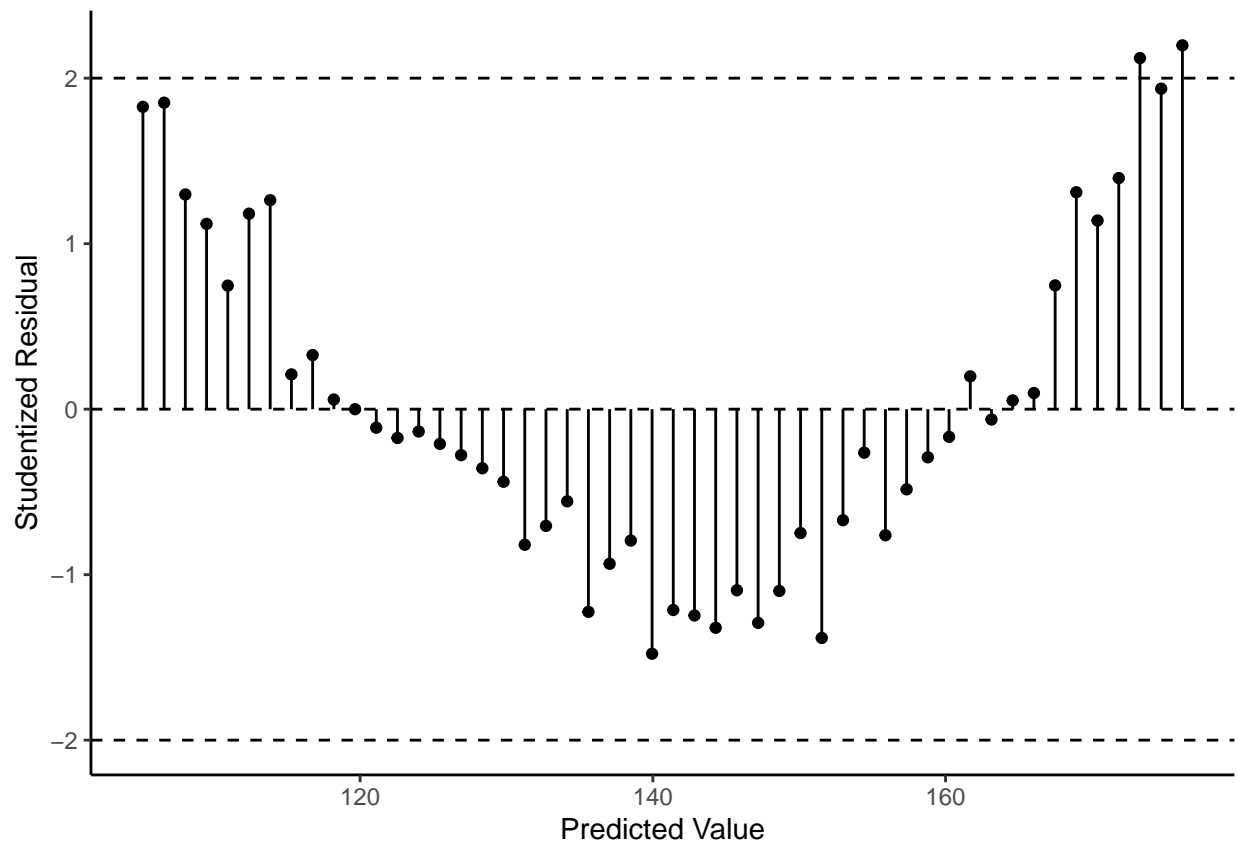
```
library(dplyr)
fakedata %>% filter(abs(rest) > 2)
```

	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?



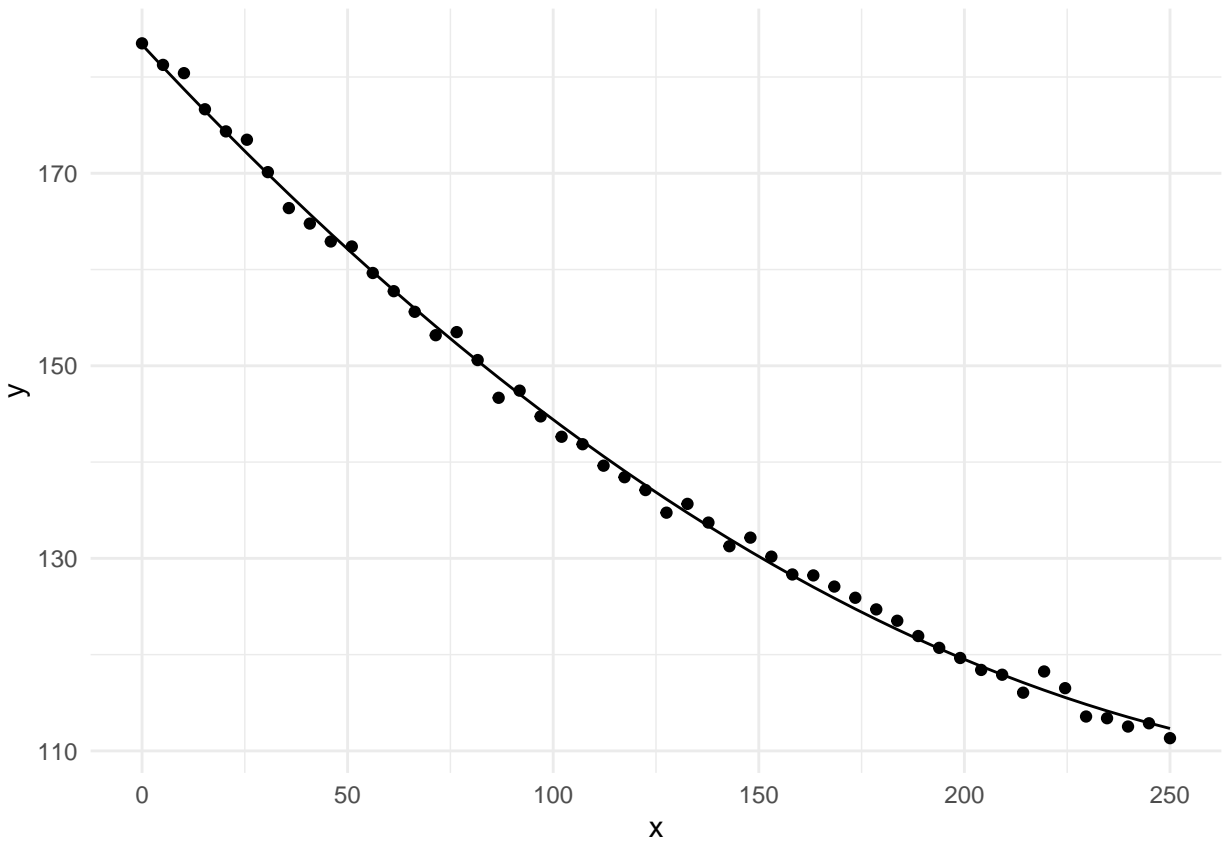
```
p <- ggplot(fakedata, aes(x = yhat, y = rest))
p <- p + geom_segment(aes(x = yhat, xend = yhat, y = 0, yend = rest))
p <- p + geom_point() + theme_classic()
p <- p + labs(x = "Predicted Value", y = "Studentized Residual")
p <- p + geom_hline(yintercept = c(-2, 0, 2), linetype = 2)
plot(p)
```



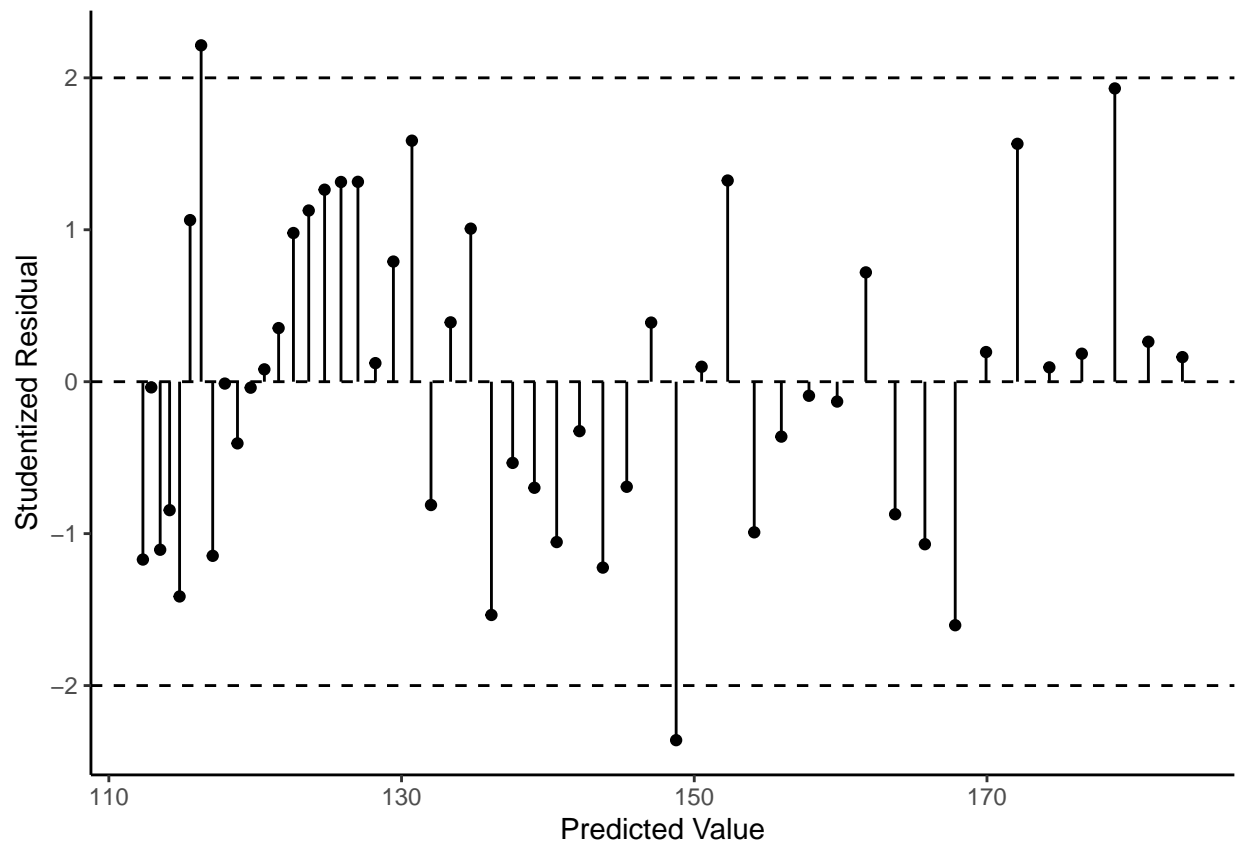
Let's try the polynomial model  $E(Y_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$ .

```
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)
```



```
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

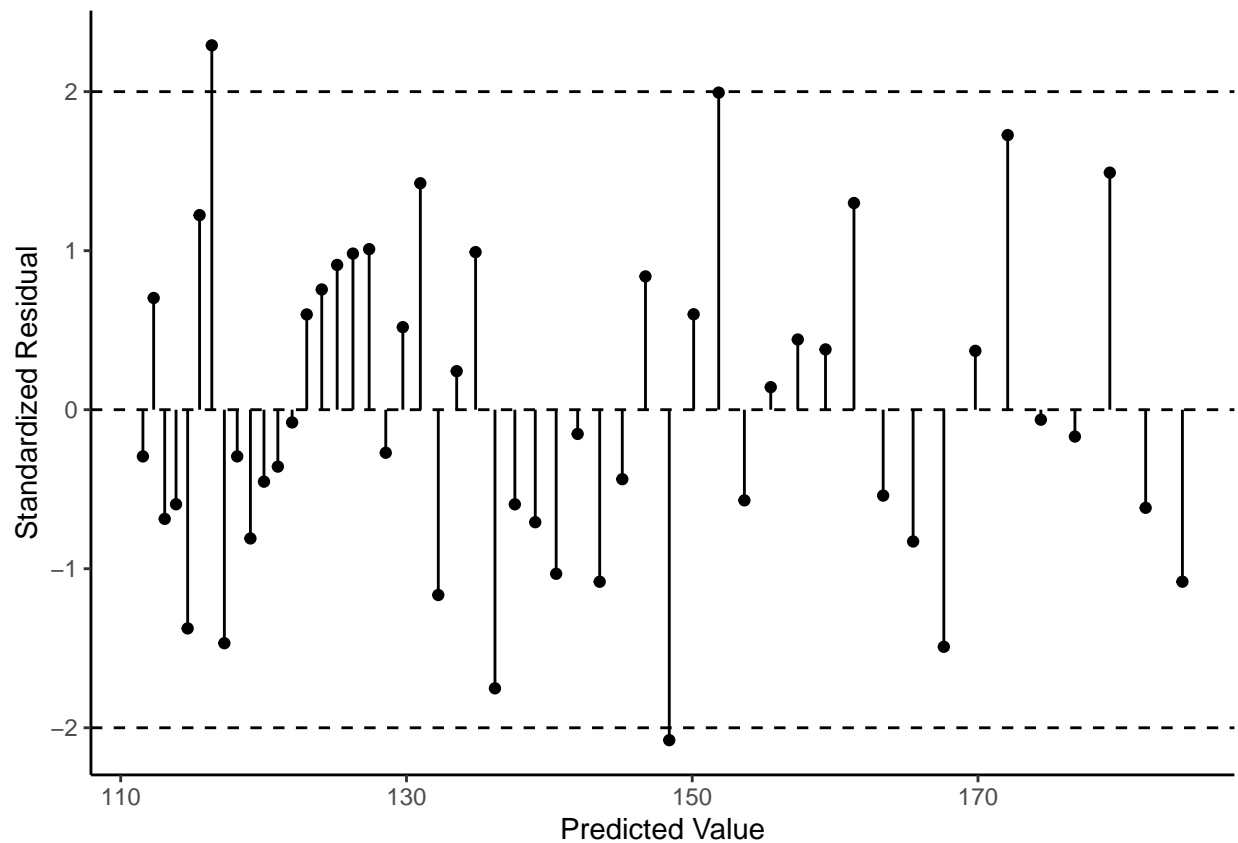
$$E(Y_i) = \alpha + (\delta - \alpha)2^{-x_i/\gamma}.$$

```
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

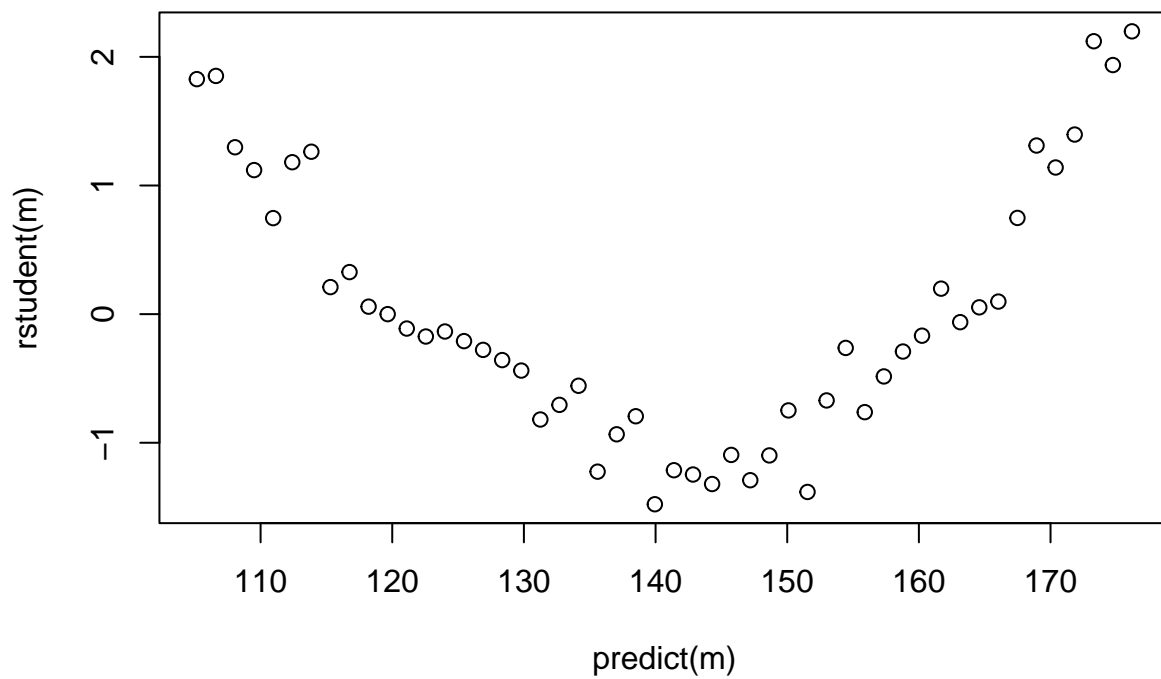
```
p <- ggplot(d, aes(x = fit, y = res)) +
  geom_segment(aes(x = fit, xend = fit, y = 0, yend = res)) +
  geom_point() + theme_classic() +
  labs(x = "Predicted Value", y = "Standardized Residual") +
  geom_hline(yintercept = c(-2, 0, 2), linetype = 2)
plot(p)
```



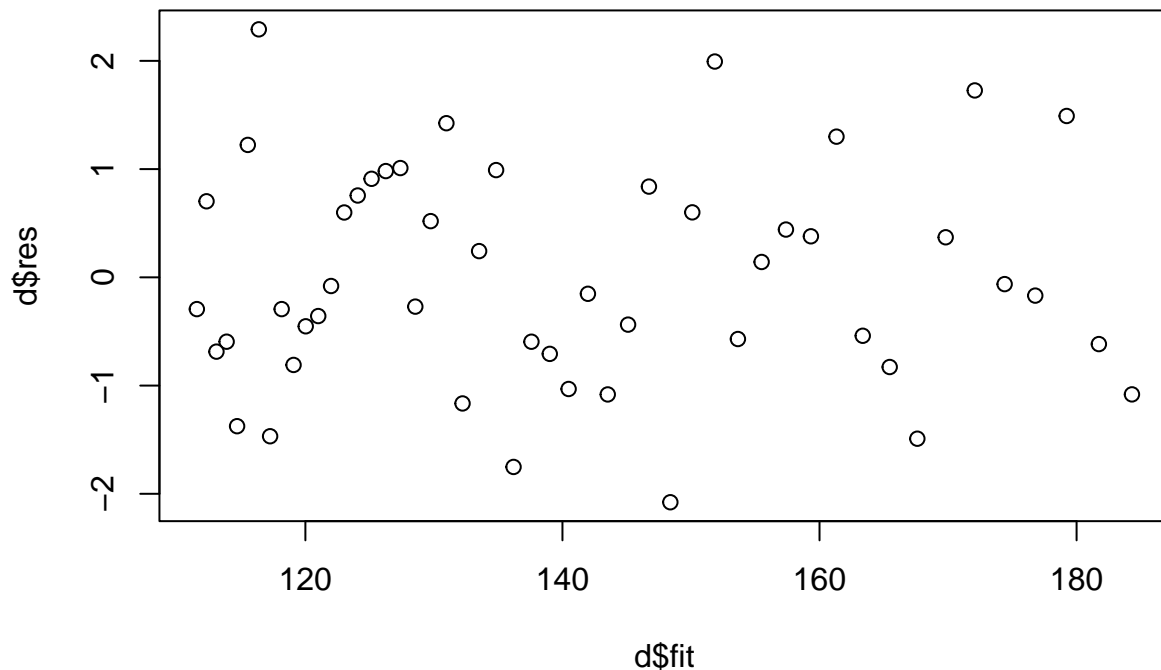


Note that since we are usually not interested in created publication quality residual plots, we can do some quick-and-dirty plots with simpler (but uglier) graphics.

```
# 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.

```
cars <- read.csv("http://webpages.uidaho.edu/~trjohns/cars.csv")
cars <- cars[,c(2,3,4,5)] # select columns 2, 3, 4, and 5
head(cars)
```

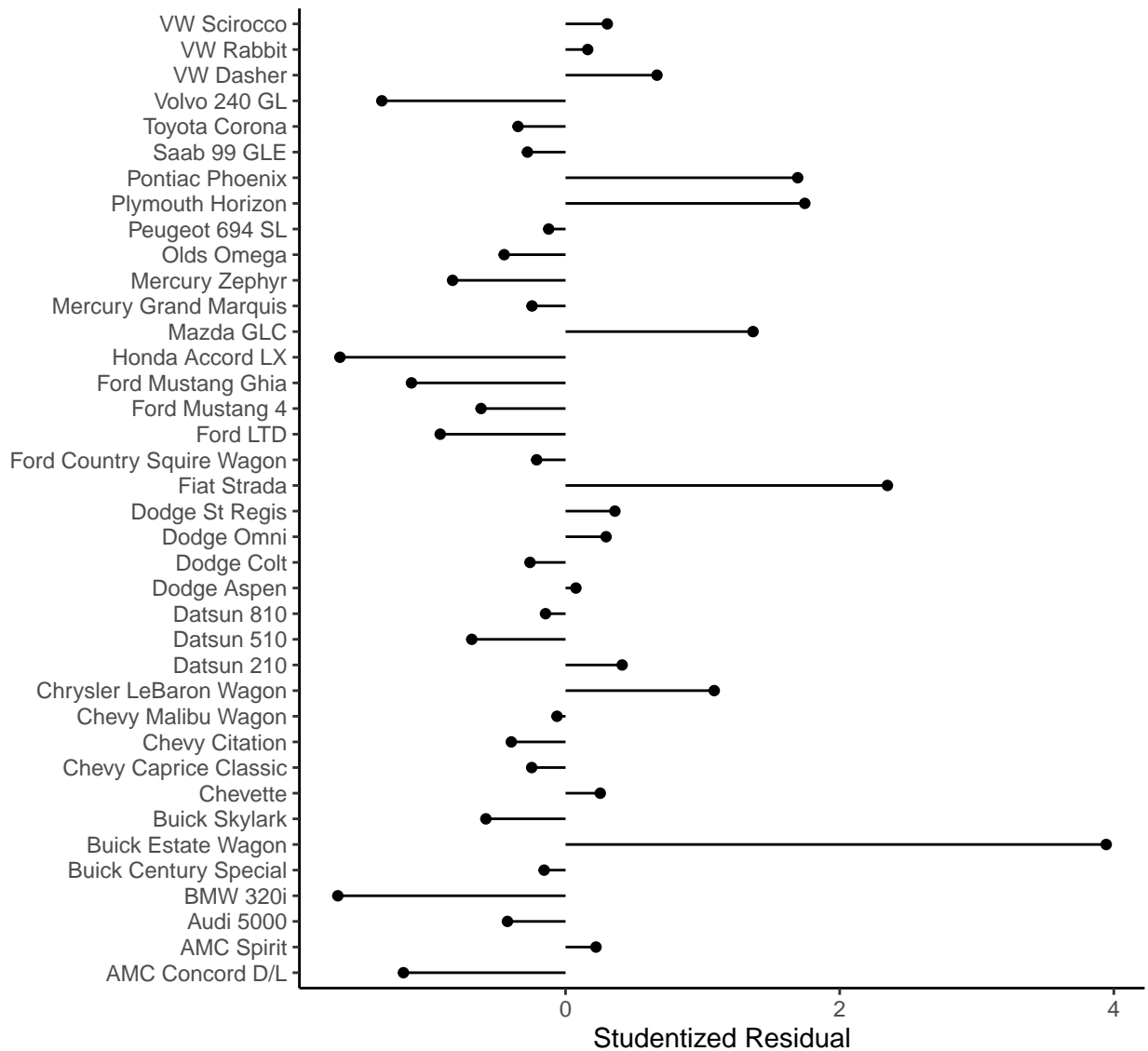
	car	mpg	weight	ratio
1	Buick Estate Wagon	16.9	4.360	2.73
2	Ford Country Squire Wagon	15.5	4.054	2.26
3	Chevy Malibu Wagon	19.2	3.605	2.56
4	Chrysler LeBaron Wagon	18.5	3.940	2.45
5	Chevette	30.0	2.155	3.70
6	Toyota Corona	27.5	2.560	3.05

```
m <- lm(mpg ~ weight + ratio, data = cars)
cars$yhat <- predict(m)
cars$rest <- rstudent(m)
subset(cars, abs(rest) > 2)
```

	car	mpg	weight	ratio	yhat	rest
1	Buick Estate Wagon	16.9	4.36	2.73	10.32	3.944
34	Fiat Strada	37.3	2.13	3.10	32.67	2.348

```
p <- ggplot(cars, aes(x = rest, y = car)) + geom_point() +
  theme_classic() +
  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 observations(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 “homoscedasticity” or sometimes “homogeneity of variance” in the context of linear models for designed experiments. A more complete description of the assumed model is

$$E(Y_i) = f(x_{i1}, x_{i2}, \dots, x_{ik}), \quad (1)$$

$$\text{Var}(Y_i) = \sigma^2. \quad (2)$$

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  $\beta_0$  term and  $k$  explanatory variables).

**Consequences:** Severe violations of homoscedasticity 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).

```
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`.

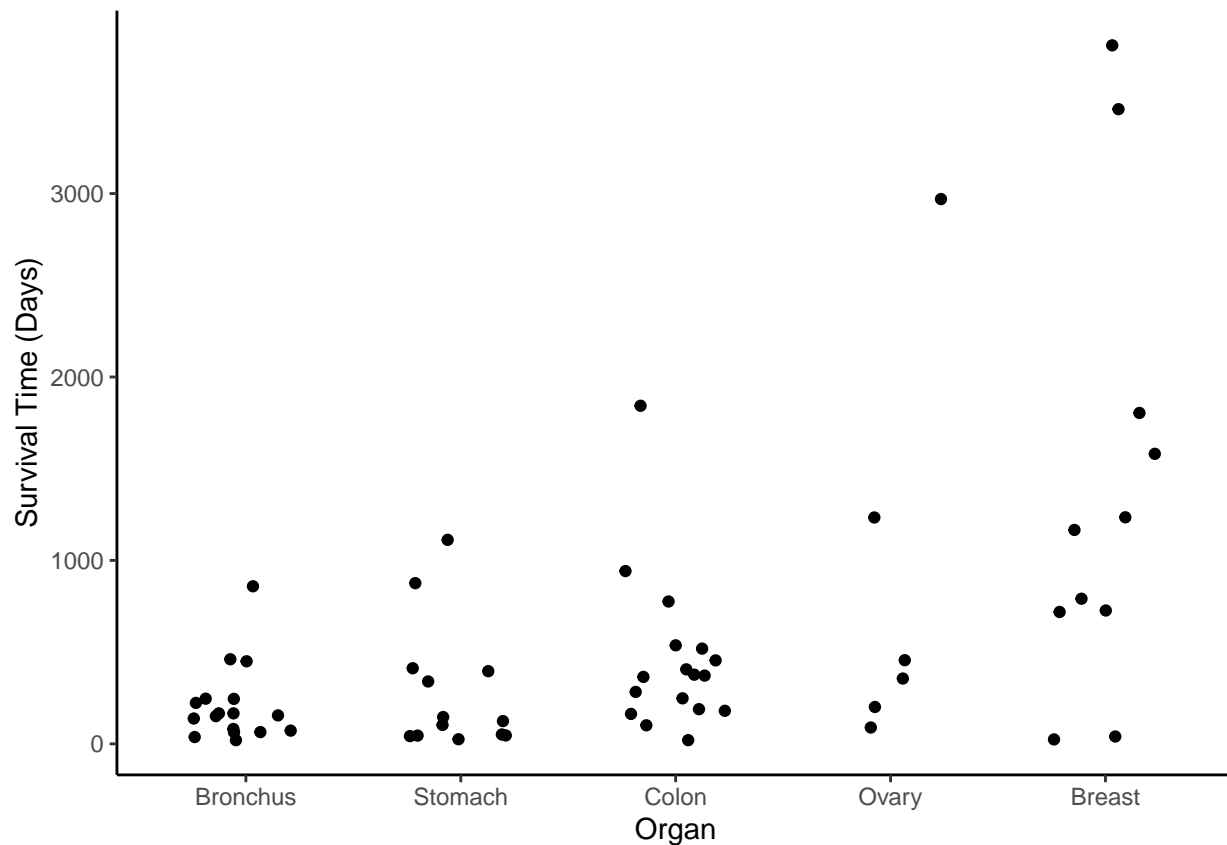
```
CancerSurvival$Organ <- with(CancerSurvival, reorder(Organ, Survival, mean))
```

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.

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

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

```
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.

```
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
```

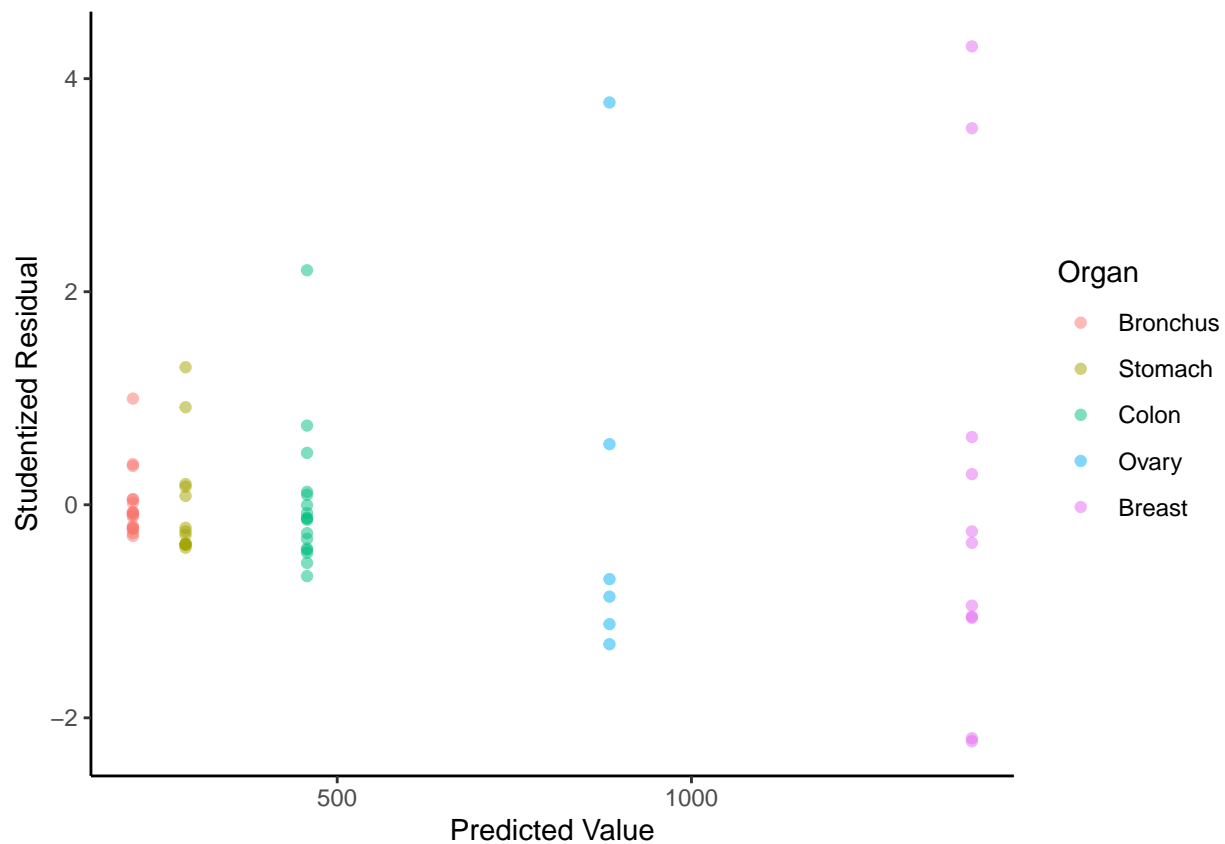
Now consider a linear model that assumes homoscedasticity.

```
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
```

```
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.

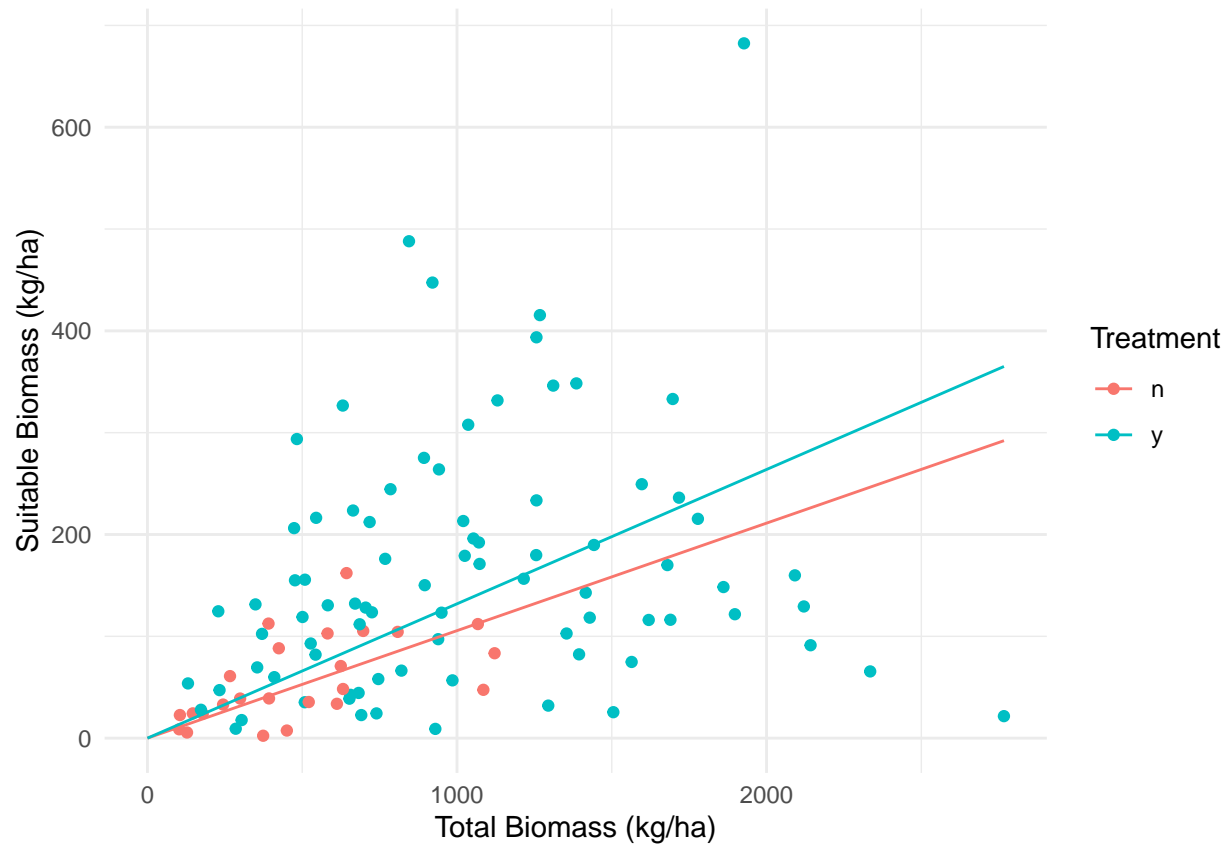
```
library(trtools) # for biomass data
```

```
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

```
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.