Friday, Feb 18

Solutions for Heteroscedasticity

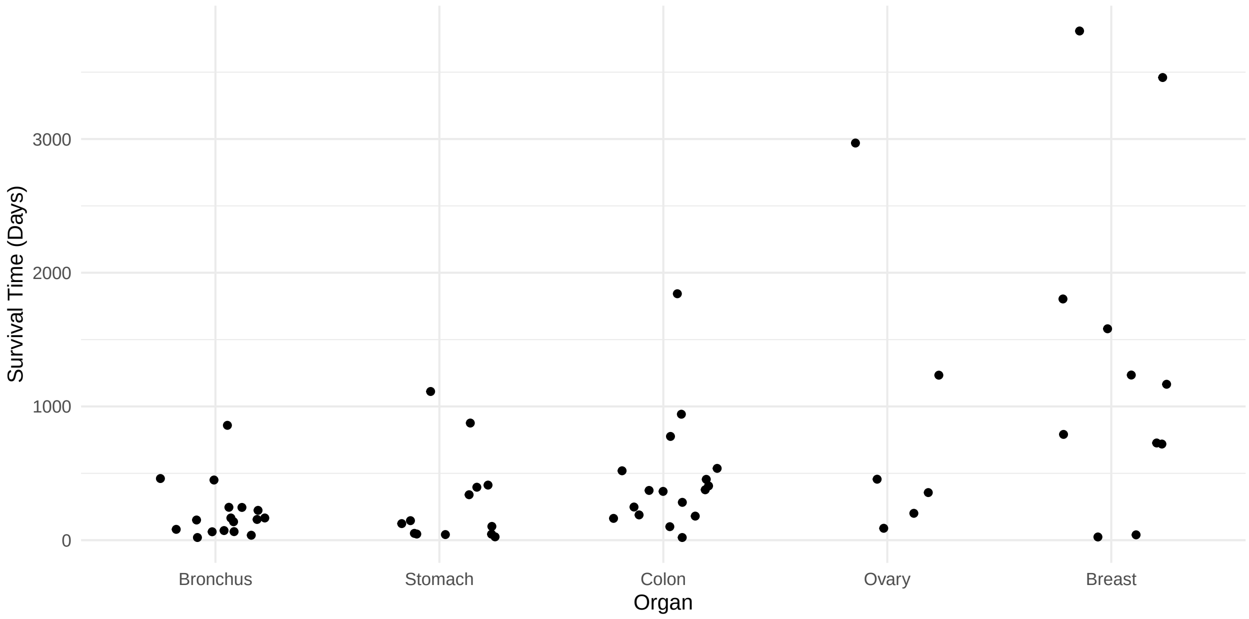
We will discuss four solutions to heteroscedasticity in linear and nonlinear regression: variance-stabilizing transformations, weighted least squares, robust standard errors, and models that do not assume homoscedasticity.

Variance-Stabilizing Transformations

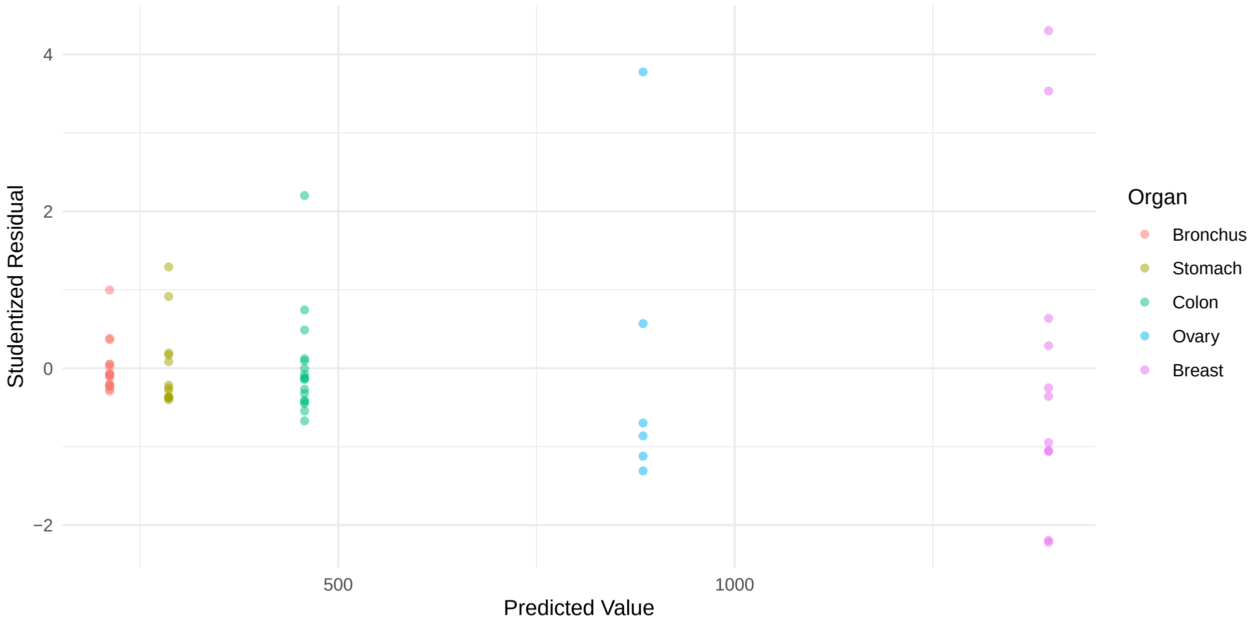
The idea is to use $Y_i^* = g(Y_i)$ instead of Y_i as the response variable, where g is a *variance-stabilizing transformation*.

Example: Consider again the cancer survival time data.

```
library(Stat2Data)
data(CancerSurvival)
CancerSurvival$Organ <- with(CancerSurvival, reorder(Organ, Survival, mean))
p <- ggplot(CancerSurvival, aes(x = Organ, y = Survival)) +
   geom_jitter(height = 0, width = 0.25) +
   labs(y = "Survival Time (Days)") + theme_minimal()
plot(p)
```

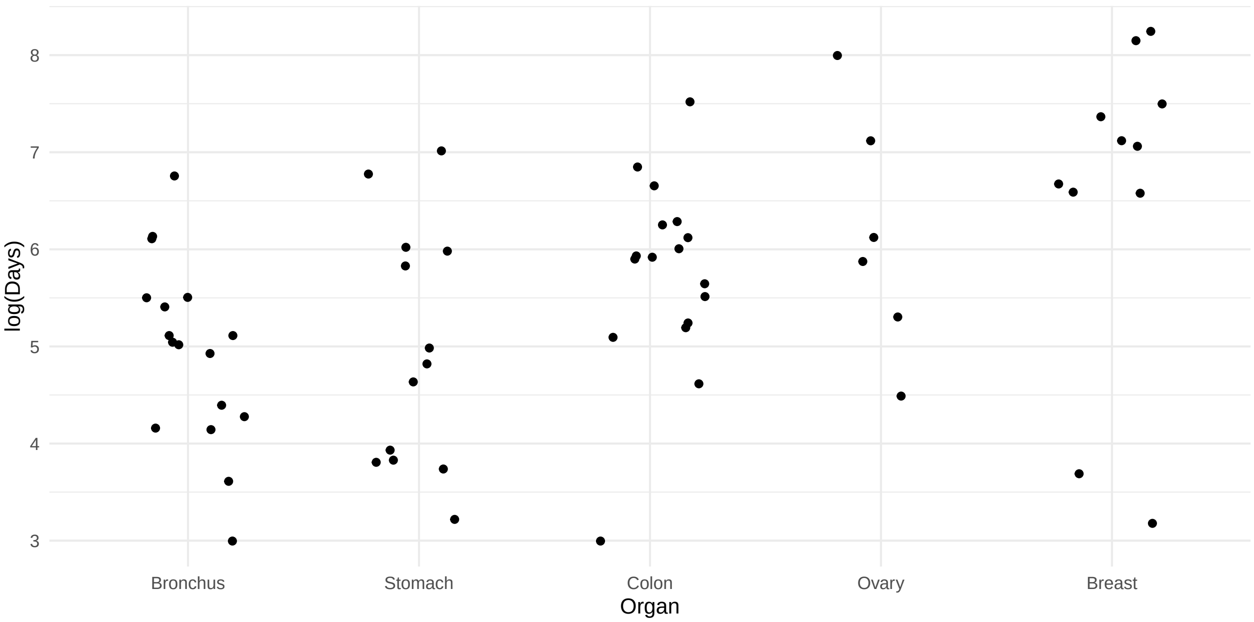


```
m <- lm(Survival ~ Organ, data = CancerSurvival)

CancerSurvival$yhat <- predict(m)
CancerSurvival$rest <- rstudent(m)

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



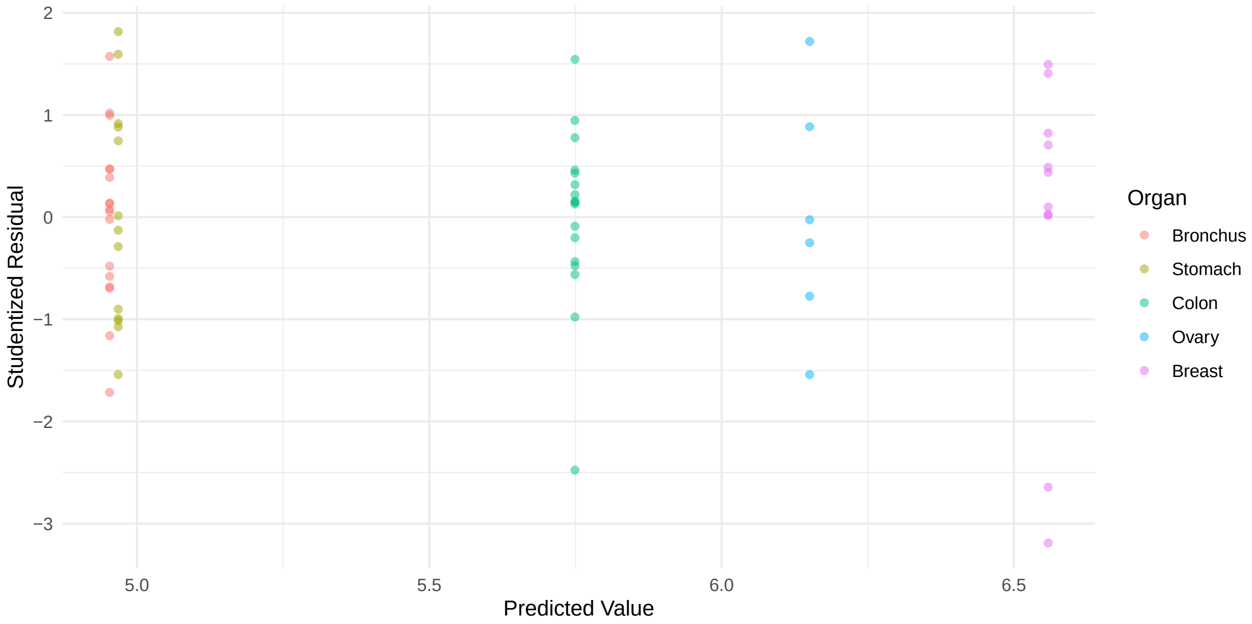
A model for *log* time might exhibit something closer to homoscedasticity.

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



```
m <- lm(log(Survival) ~ Organ, data = CancerSurvival)
```

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

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



Comments on variance-stabilizing transformations.

1. Depending on the situation, other transformations may exhibit variance-stabilizing properties. Some common transformations are $\sqrt{Y_i}$, $\log(Y_i)$, $1/\sqrt{Y_i}$ and $1/Y_i$ for right-skewed response variables, and $n_i \sin^{-1}\sqrt{Y_i}$ when Y_i is a proportion with a denominator of n_i.

2. A limitation of variance stabilizing transformations is that it is often difficult (and undesirable) to to *interpret* the model in terms of the transformed response variable (although there are exceptions as we will later see with the log transformation in the context of accelerated failure time models for survival data).

3. It is important to note that for any *nonlinear* transformation that $E[g(Y)] \neq g[E(Y)]$ (i.e., the expected transformed response does not necessarily equal the transformed expected response). For example, the expected log of survival time does not equal the log of the expected survival time. So we cannot obtain inferences for the expected response by applying the inverse function. For example, while we have that $\exp[\log(Y)] = Y$, this **does not** imply that $\exp\{E[\log(Y)]\} = E(Y)$.

Weighted Least Squares

A *weighted* least squares (WLS) estimator of the regression model parameters minimizes

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

were $w_i > 0$ is the *weight* for the i-th observation. So-called *ordinary least squares* (OLS) or *unweighted least squares* is a special case where all $w_i = 1$.

To account for heteroscedasticity, the weights should be *inversely proportional to the variance of the response* so that

$$w_i \propto \frac{1}{\text{Var}(Y_i)}.$$

Estimation is *efficient* meaning that the *true* standard errors (which are not necessarily the *reported* standard errors shown by software since these are estimates and may be biased without using weights as defined above) are as small as they can be when using weighted least squares.

Example: One situation where we can anticipate heteroscedasticity and the need for weights is when the response variable is the mean of a varying number of observations. Consider the following data.

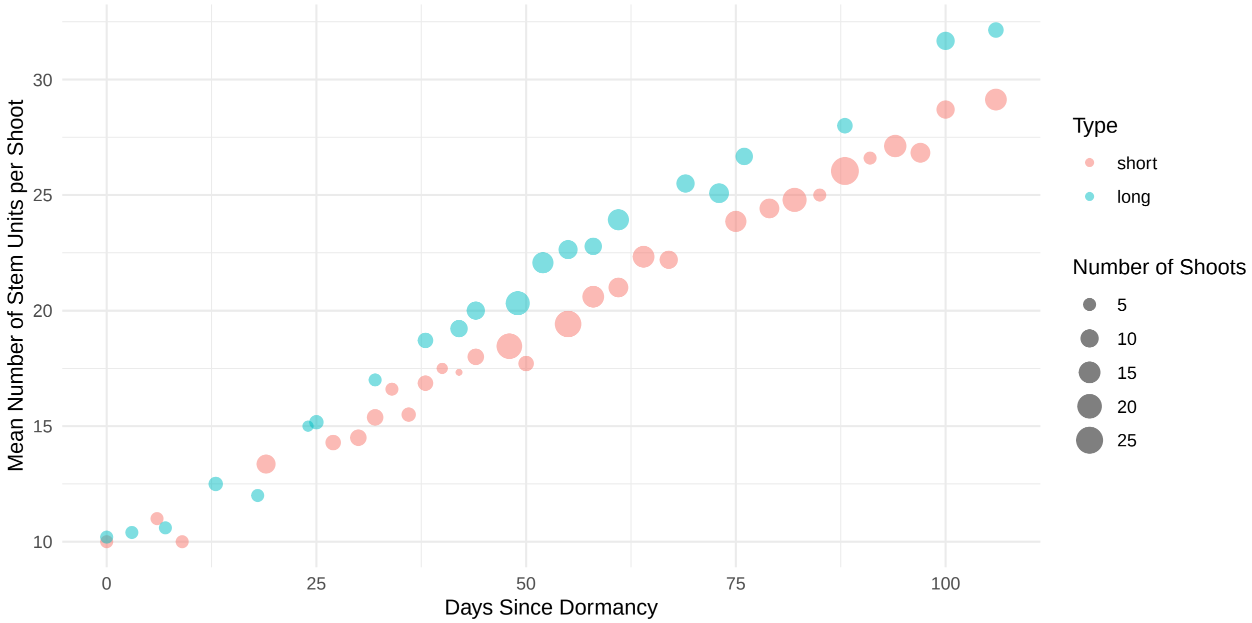
```r
library(alr4)
head(allshoots)
```

```
  Day  n  ybar   SD Type
1   0  5 10.00 0.00    0
2   6  5 11.00 0.72    0
3   9  5 10.00 0.72    0
4  19 11 13.36 1.03    0
5  27  7 14.29 0.95    0
6  30  8 14.50 1.19    0
```

```r
allshoots$Type <- factor(allshoots$Type, labels = c("short","long"))
head(allshoots)
```

```
  Day  n  ybar   SD  Type
1   0  5 10.00 0.00 short
2   6  5 11.00 0.72 short
3   9  5 10.00 0.72 short
4  19 11 13.36 1.03 short
5  27  7 14.29 0.95 short
6  30  8 14.50 1.19 short
```

```r
p <- ggplot(allshoots, aes(x = Day, y = ybar, size = n, color = Type)) +
   geom_point(alpha = 0.5) + theme_minimal() +
   labs(x = "Days Since Dormancy",
      y = "Mean Number of Stem Units per Shoot",
      size = "Number of Shoots")
plot(p)
```



The response variable is an *mean* of several observations so that

$$Y_i = \frac{Z_{i1} + Z_{i2} + \cdots + Z_{in_i}}{n_i}$$

where Z_{ij} is the length of the j-th shoot that goes into the i-th average, and a total of n_i shoots go into the i-th average. If $\text{Var}(Z_{ij}) = \sigma^2$ then $\text{Var}(Y_i) = \sigma^2/n_i$. Thus the weights should be

$$w_i \propto \frac{1}{\sigma^2/n_i} = \frac{n_i}{\sigma^2}.$$

Since $1/\sigma^2$ is a constant for all observations, we can define the weights as $w_i = n_i$. The weights can be specified in `lm` and `nls` (and other functions for regression) using the `weights` argument.

```
# weighted least squares
m <- lm(ybar ~ Type + Day + Type:Day, weights = n, data = allshoots)
cbind(summary(m)$coefficients, confint(m))
```

```
             Estimate Std. Error t value  Pr(>|t|)    2.5 %
(Intercept)   9.48837   0.238615  39.764 2.126e-38  9.00861
Typelong      0.48538   0.362496   1.339 1.869e-01 -0.24347
Day           0.18726   0.003486  53.722 1.559e-44  0.18025
Typelong:Day  0.03007   0.005800   5.185 4.281e-06  0.01841
              97.5 %
(Intercept)  9.96814
Typelong     1.21423
Day          0.19427
Typelong:Day 0.04173
```

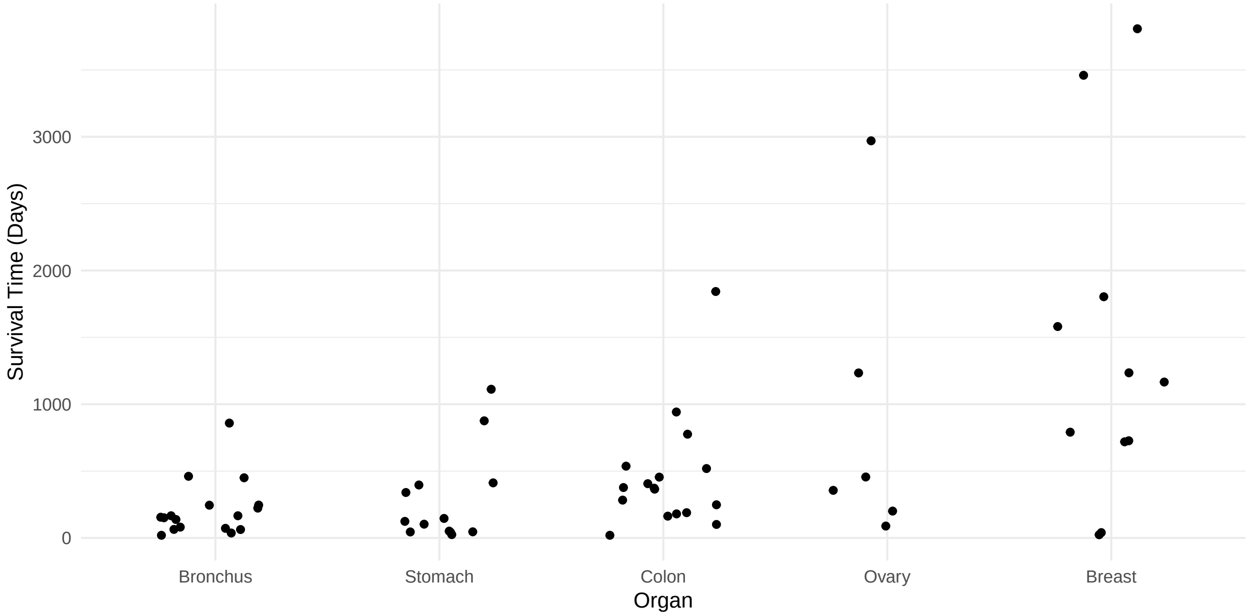
```
trtools::contrast(m,
  a = list(Type = c("short","long"), Day = 1),
  b = list(Type = c("short","long"), Day = 0),
  cnames = c("short shoot slope","long shoot slope"))
```

```
                  estimate       se  lower  upper tvalue df
short shoot slope   0.1873 0.003486 0.1802 0.1943  53.72 48
long shoot slope    0.2173 0.004636 0.2080 0.2267  46.88 48
```

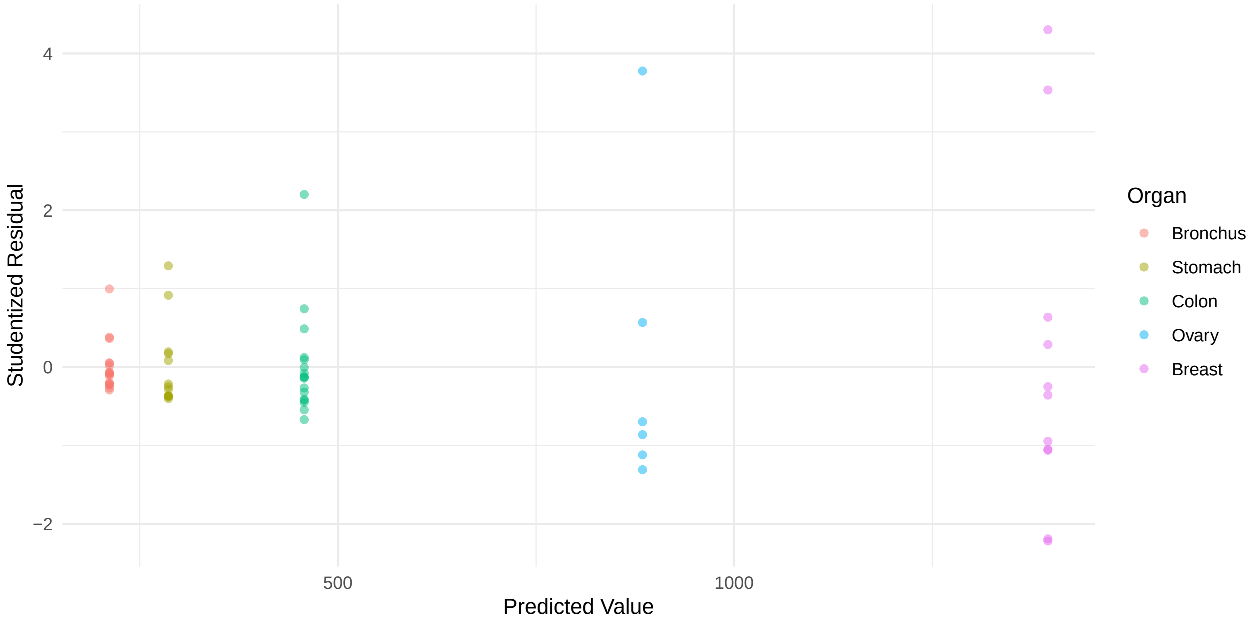
```
                        pvalue
short shoot slope 1.559e-44
long shoot slope  9.535e-42
```

Example: Consider again the cancer survival time data.

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



```
m.ols <- lm(Survival ~ Organ, data = CancerSurvival)

CancerSurvival$yhat <- predict(m.ols)
CancerSurvival$rest <- rstudent(m.ols)

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



There are a couple of ways we could go with these data. One is that since we have a categorical explanatory variable with multiple observations per category, we could *estimate* the variance of Y_i of each organ, and then set the weights to the reciprocals of these estimated variances.

```
library(dplyr)
CancerSurvival %>% group_by(Organ) %>%
  summarize(variance = var(Survival), weight = 1/var(Survival))
```

```
# A tibble: 5 x 3
  Organ    variance      weight
  <fct>       <dbl>       <dbl>
1 Bronchus   44041. 0.0000227
2 Stomach   119930. 0.00000834
3 Colon     182473. 0.00000548
4 Ovary    1206875. 0.000000829
5 Breast   1535038. 0.000000651
```

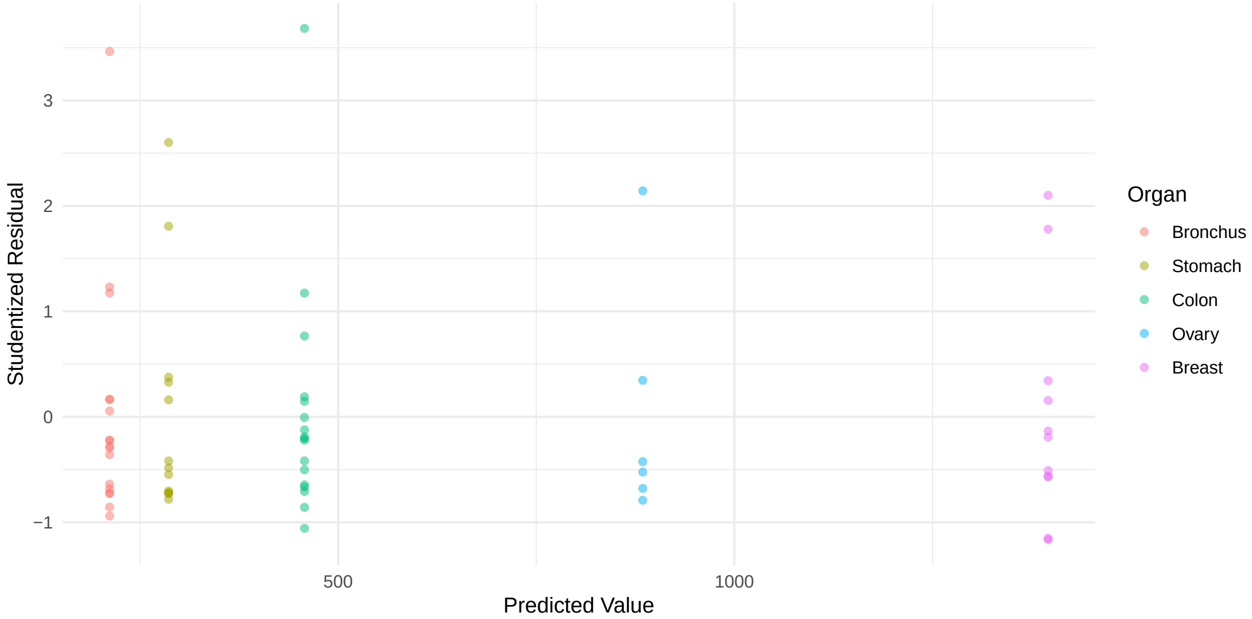
We can use the following to compute weights and add them to the data frame.

```
CancerSurvival <- CancerSurvival %>%
   group_by(Organ) %>% mutate(w = 1/var(Survival))
head(CancerSurvival)
```

```
# A tibble: 6 x 3
# Groups:   Organ [1]
  Survival Organ            w
     <int> <fct>        <dbl>
1      124 Stomach 0.00000834
2       42 Stomach 0.00000834
3       25 Stomach 0.00000834
4       45 Stomach 0.00000834
5      412 Stomach 0.00000834
6       51 Stomach 0.00000834
```

Now let's estimate the model using weighted least squares with these weights and inspect the residuals.

```r
m.wls <- lm(Survival ~ Organ, weights = w, data = CancerSurvival)

CancerSurvival$yhat <- predict(m.wls)
CancerSurvival$rest <- rstudent(m.wls)

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



Note how this affects our inferences.

```r
cbind(summary(m.ols)$coefficients, confint(m.ols))
```

```
             Estimate Std. Error t value  Pr(>|t|)   2.5 %
(Intercept)    211.59      162.4  1.3030 0.1976373 -113.34
OrganStomach    74.41      246.7  0.3017 0.7639784 -419.20
OrganColon     245.82      229.6  1.0704 0.2887820 -213.70
OrganOvary     672.75      317.9  2.1160 0.0385749   36.56
OrganBreast   1184.32      259.1  4.5713 0.0000253  665.91
             97.5 %
(Intercept)   536.5
OrganStomach  568.0
OrganColon    705.3
OrganOvary   1308.9
OrganBreast  1702.7
```

```r
cbind(summary(m.wls)$coefficients, confint(m.wls))
```

```
             Estimate Std. Error t value  Pr(>|t|)   2.5 %
(Intercept)    211.59       50.9  4.1571 0.0001057  109.74
OrganStomach    74.41      108.7  0.6846 0.4963078 -143.10
OrganColon     245.82      115.4  2.1296 0.0373858   14.85
OrganOvary     672.75      451.4  1.4904 0.1414343 -230.45
```

```
OrganBreast   1184.32      377.0  3.1413 0.0026291  429.92
             97.5 %
(Intercept)   313.4
OrganStomach  291.9
OrganColon    476.8
OrganOvary   1575.9
OrganBreast  1938.7
```

```
organs <- unique(CancerSurvival$Organ)
trtools::contrast(m.ols, a = list(Organ = organs), cnames = organs)
```

```
         estimate    se   lower  upper tvalue df    pvalue
Stomach     286.0 185.7  -85.57  657.6  1.540 59 1.289e-01
Bronchus    211.6 162.4 -113.34  536.5  1.303 59 1.976e-01
Colon       457.4 162.4  132.48  782.3  2.817 59 6.587e-03
Ovary       884.3 273.3  337.39 1431.3  3.235 59 1.993e-03
Breast     1395.9 201.9  991.96 1799.9  6.915 59 3.770e-09
```

```
trtools::contrast(m.wls, a = list(Organ = organs), cnames = organs)
```

```
         estimate     se  lower  upper tvalue df    pvalue
Stomach     286.0  96.05  93.81  478.2  2.978 59 0.0042091
Bronchus    211.6  50.90 109.74  313.4  4.157 59 0.0001057
Colon       457.4 103.60 250.10  664.7  4.415 59 0.0000437
Ovary       884.3 448.49 -13.10 1781.8  1.972 59 0.0533281
Breast     1395.9 373.56 648.41 2143.4  3.737 59 0.0004228
```

```
trtools::contrast(m.ols,
   a = list(Organ = "Breast"),
   b = list(Organ = c("Bronchus","Stomach","Colon","Ovary")),
   cnames = c("Breast vs Bronchus", "Breast vs Stomach",
      "Breast vs Colon","Breast vs Ovary"))
```

```
                   estimate    se  lower upper tvalue df
Breast vs Bronchus   1184.3 259.1  665.9  1703  4.571 59
Breast vs Stomach    1109.9 274.3  561.1  1659  4.046 59
Breast vs Colon       938.5 259.1  420.1  1457  3.622 59
Breast vs Ovary       511.6 339.8 -168.4  1192  1.506 59
                      pvalue
Breast vs Bronchus 0.0000253
Breast vs Stomach  0.0001533
Breast vs Colon    0.0006083
Breast vs Ovary    0.1375263
```

```
trtools::contrast(m.wls,
   a = list(Organ = "Breast"),
   b = list(Organ = c("Bronchus","Stomach","Colon","Ovary")),
   cnames = c("Breast vs Bronchus", "Breast vs Stomach",
      "Breast vs Colon","Breast vs Ovary"))
```

```
                   estimate    se  lower upper tvalue df
Breast vs Bronchus   1184.3 377.0  429.9  1939 3.1413 59
Breast vs Stomach    1109.9 385.7  338.1  1882 2.8776 59
Breast vs Colon       938.5 387.7  162.8  1714 2.4209 59
Breast vs Ovary       511.6 583.7 -656.4  1680 0.8765 59
                     pvalue
Breast vs Bronchus 0.002629
Breast vs Stomach  0.005572
Breast vs Colon    0.018577
Breast vs Ovary    0.384340
```

Here's how you can do the comparison of one level with all others using the `contrast` function from the **emmeans** package.

```
library(emmeans)
contrast(emmeans(m.wls, ~ Organ), "trt.vs.ctrl", ref = "Breast",
   reverse = TRUE, adjust = "none", infer = TRUE)
```

```
 contrast          estimate  SE df lower.CL upper.CL
 Breast - Bronchus     1184 377 59      430     1939
 Breast - Stomach      1110 386 59      338     1882
 Breast - Colon         938 388 59      163     1714
 Breast - Ovary         512 584 59     -656     1680
 t.ratio p.value
   3.141  0.0026
   2.878  0.0056
   2.421  0.0186
   0.876  0.3843

Confidence level used: 0.95
```

Another approach is to assume that the variance of the response variable is some function of its expected response, and thus the weights are a function of the expected response. With right-skewed response variables one common functional relationship is that

$$\text{Var}(Y_i) \propto E(Y_i),$$

or, more generally,

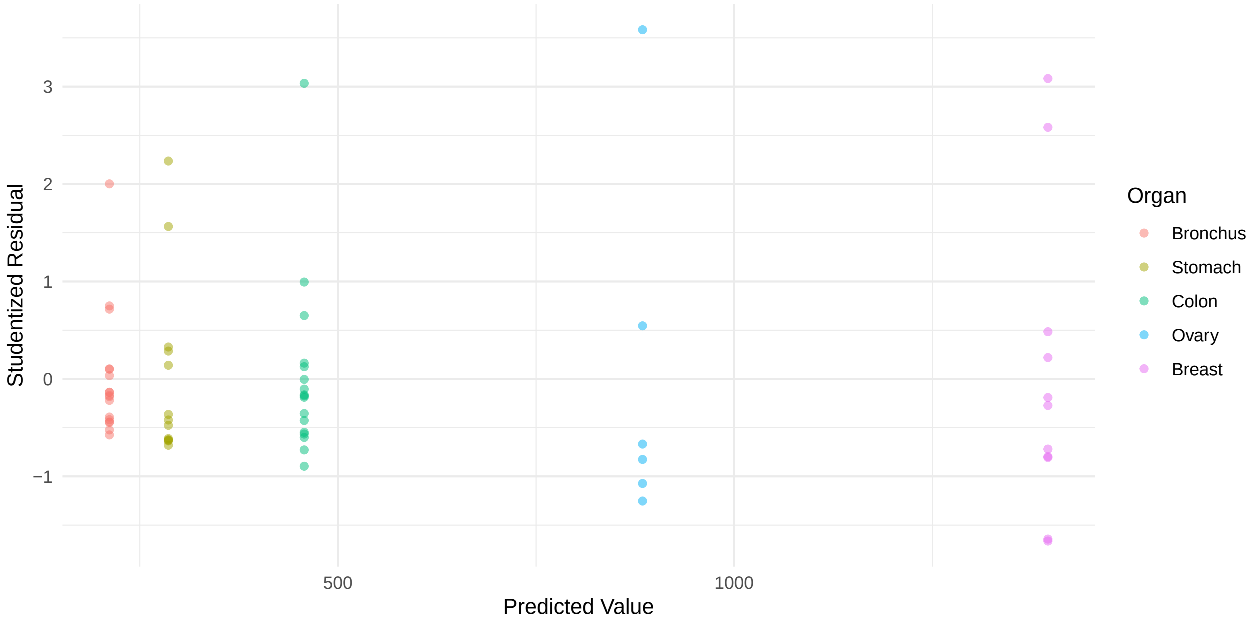
$$\text{Var}(Y_i) \propto E(Y_i)^p,$$

where p is some power (usually $p \geq 1$). So the weights would then be

$$w_i \propto \frac{1}{E(Y_i)^p}.$$

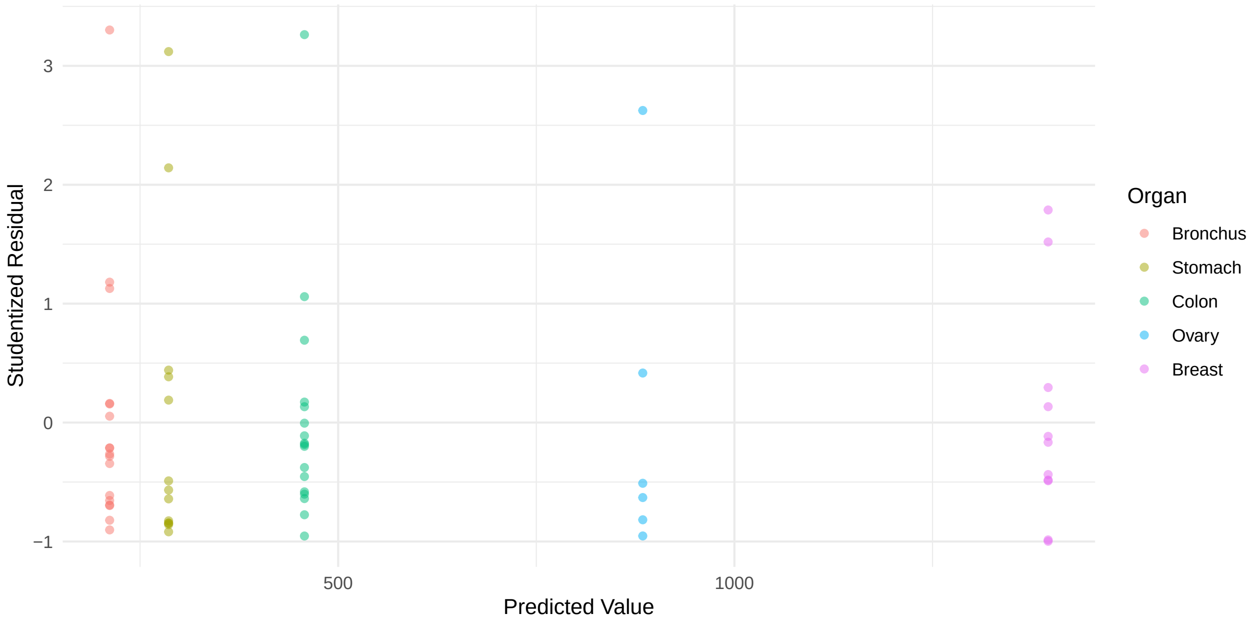
We do not know $E(Y_i)$, but $\hat{y}_i$ is an estimate of $E(Y_i)$. Since $\hat{y}_i$ does not depend on the weights for the model for the `CancerSurvival` data we can use the estimates from ordinary least squares to obtain weights of $w_i = 1/\hat{y}_i^p$.

```
m.ols <- lm(Survival ~ Organ, data = CancerSurvival)

CancerSurvival$w <- 1/predict(m.ols)
m.wls <- lm(Survival ~ Organ, data = CancerSurvival, weights = w)

CancerSurvival$yhat <- predict(m.wls)
CancerSurvival$rest <- rstudent(m.wls)

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



Maybe we could do better. Let's try $p = 2$ — i.e., $\text{Var}(Y_i) \propto E(Y_i)^2$.

```
m.ols <- lm(Survival ~ Organ, data = CancerSurvival)

CancerSurvival$w <- 1/predict(m.ols)^2
m.wls <- lm(Survival ~ Organ, data = CancerSurvival, weights = w)

CancerSurvival$yhat <- predict(m.wls)
CancerSurvival$rest <- rstudent(m.wls)

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

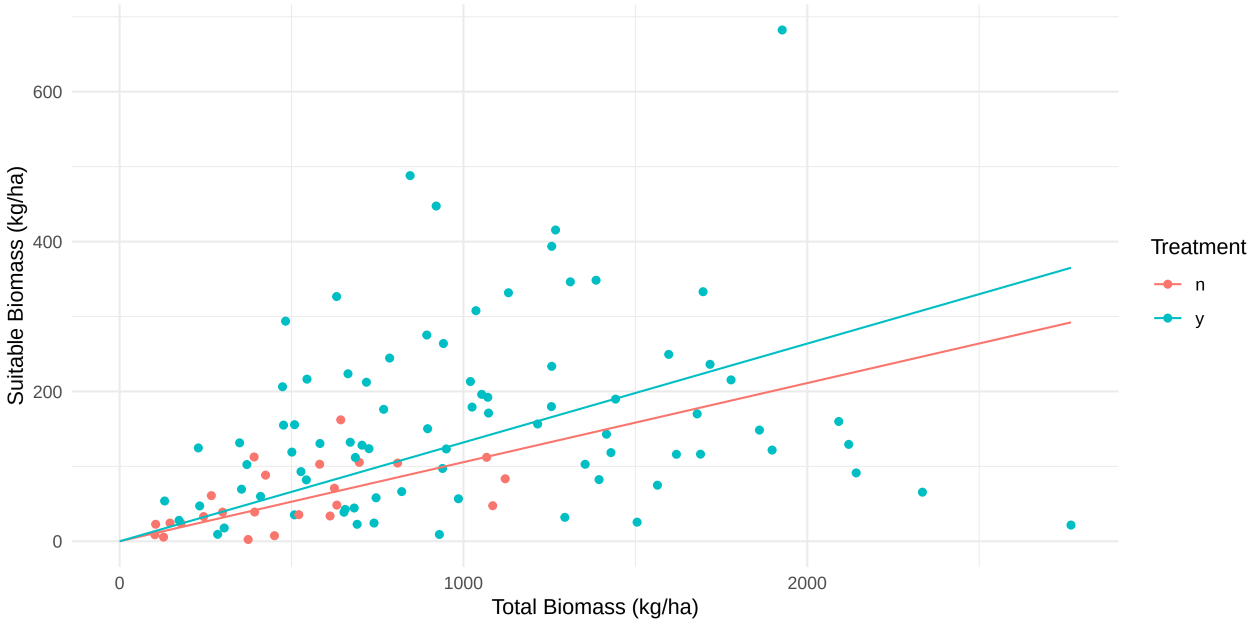


Example: Consider again following data from a study on the effects of fuel reduction on biomass.

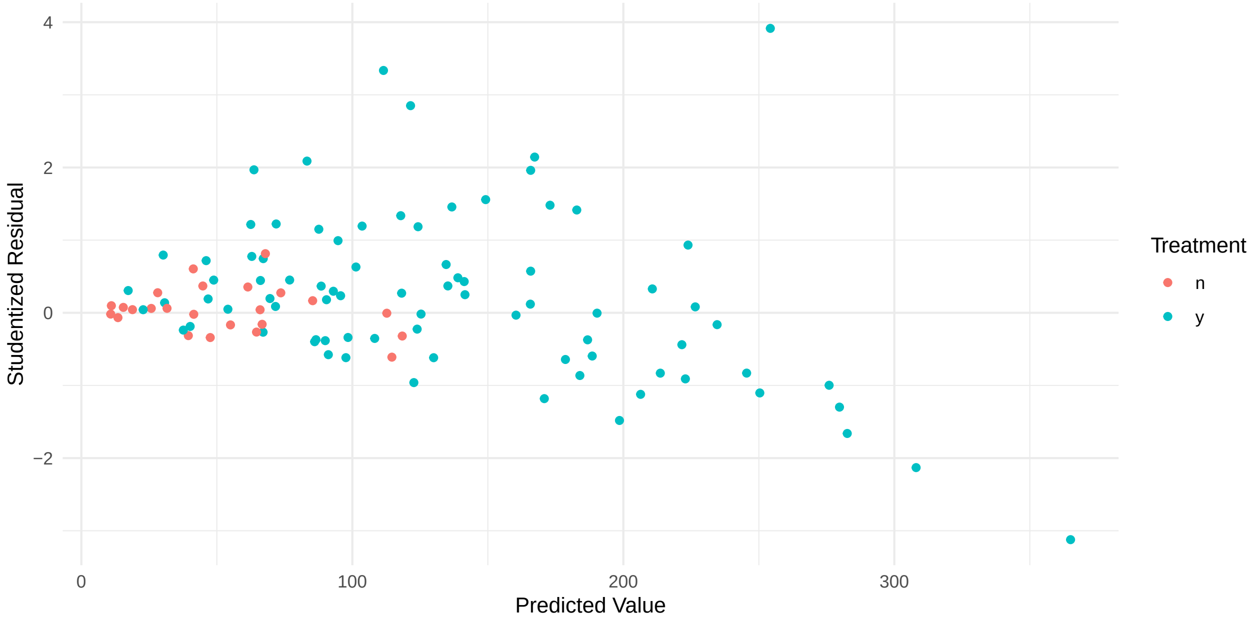
```
library(trtools) # for biomass data

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)
```



Here we might also assume that $\text{Var}(Y_i) \propto E(Y_i)^p$, with weights of $w_i = 1/\hat{y}_i$. But here things are a bit more complicated for this model: the w_i depend on the $\hat{y}_i$, the $\hat{y}_i$ depend on the w_i. In the model for the `CancerSurvival` data this was not an issue because there the estimates of the model parameters, and thus

$\hat{y}_i$, did not depend on the weights so we could use ordinary least squares where all $w_i = 1$ to get the $\hat{y}_i$. But that is not true for this model. But we can solve this problem using *iteratively weighted least squares*.