Wednesday, January 29

The Estimated Expected Response

Assuming the linear model

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k,$$

the estimated expected response at specified values of the response variables is

$$\widehat{E(Y)} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_k x_k,$$

where $x_1, x_2, \dots, x_k$ are specified values of the explanatory variables. Because $\widehat{E(Y)}$ is sometimes used for *predicting* Y, we sometimes refer to it as the "predicted value" of Y and denote it as $\hat{y}$.

Note that an expected response is simply a linear combination of the form

$$\ell = a_0\beta_0 + a_1\beta_1 + a_2\beta_2 + \cdots + a_k\beta_k + b,$$

where $a_0 = 1, a_1 = x_1, a_2 = x_2, \dots, a_k = x_k$ and $b = 0$.

Example: Consider the following model for the `whiteside` data.

```
m <- lm(Gas ~ Insul + Temp + Insul:Temp, data = MASS::whiteside) # note :: operator
summary(m)$coefficients
```

```
                Estimate Std. Error t value  Pr(>|t|)
(Intercept)       6.8538    0.13596  50.409 7.997e-46
InsulAfter       -2.1300    0.18009 -11.827 2.316e-16
Temp             -0.3932    0.02249 -17.487 1.976e-23
InsulAfter:Temp   0.1153    0.03211   3.591 7.307e-04
```

What is the estimated expected gas consumption at 0, 5, and 10 degrees C after insulation? Either `lincon` or `contrast` can be used (although `contrast` is probably easier).

```
library(trtools)
lincon(m, a = c(1,1,0,0))   # After @ 0C
```

```
            estimate     se lower upper tvalue df    pvalue
(1,1,0,0),0    4.724 0.1181 4.487 4.961     40 52 9.918e-41
```

```
lincon(m, a = c(1,1,5,5))   # After @ 5C
```

```
            estimate      se lower upper tvalue df    pvalue
(1,1,5,5),0    3.334 0.06024 3.213 3.455  55.35 52 6.772e-48
```

```
lincon(m, a = c(1,1,10,10)) # After @ 10C
```

```
              estimate   se lower upper tvalue df    pvalue
(1,1,10,10),0    1.945 0.14 1.664 2.225  13.89 52 3.869e-19
```

```
contrast(m, a = list(Insul = "After", Temp = c(0,5,10)),
  cnames = c("After @ 0C","After @ 5C","After @ 10C"))
```

```
            estimate      se lower upper tvalue df    pvalue
After @ 0C     4.724 0.11810 4.487 4.961  40.00 52 9.918e-41
```

```
After @ 5C      3.334 0.06024 3.213 3.455  55.35 52 6.772e-48
After @ 10C     1.945 0.13996 1.664 2.225  13.89 52 3.869e-19
```

There are better approaches if we want more points.

```r
d <- expand.grid(Temp = c(0,5,10), Insul = c("Before","After"))
d
```

```
  Temp  Insul
1    0 Before
2    5 Before
3   10 Before
4    0  After
5    5  After
6   10  After
```

```r
predict(m, newdata = d)
```

```
    1     2     3     4     5     6 
6.854 4.888 2.921 4.724 3.334 1.945 
```

```r
predict(m, newdata = d, interval = "confidence")
```

```
    fit   lwr   upr
1 6.854 6.581 7.127
2 4.888 4.760 5.016
3 2.921 2.676 3.167
4 4.724 4.487 4.961
5 3.334 3.213 3.455
6 1.945 1.664 2.225
```

```r
cbind(d, predict(m, newdata = d, interval = "confidence"))
```

```
  Temp  Insul   fit   lwr   upr
1    0 Before 6.854 6.581 7.127
2    5 Before 4.888 4.760 5.016
3   10 Before 2.921 2.676 3.167
4    0  After 4.724 4.487 4.961
5    5  After 3.334 3.213 3.455
6   10  After 1.945 1.664 2.225
```

Prediction and the Standard Error of Prediction

The estimated expected response $\widehat{E(Y)}$ can also be viewed as the *predicted value* of Y, justified by least squares. The estimate of Y is then

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_k x_k.$$

The (estimated) standard deviation of $Y - \hat{Y}$ is the *standard error of prediction*, defined as

$$\text{SE}(\hat{Y} - Y) = \sqrt{\text{SE}(\hat{Y})^2 + \sigma^2},$$

where σ^2 is the variance of Y (note *two* sources of variability — that of $\hat{Y}$ and that of Y). The *prediction interval* for Y is then

$$\hat{y} \pm t\sqrt{\text{SE}(\hat{Y})^2 + \sigma^2}.$$

Compare this with the confidence interval for $\widehat{E(Y)}$ which is

$$\hat{y} \pm t\text{SE}(\hat{Y}).$$

Prediction intervals for Y are wider than confidence intervals for $E(Y)$.

Example: Prediction intervals for `lm` objects can also be obtained form `predict`.

```
predict(m, newdata = d, interval = "prediction")
```

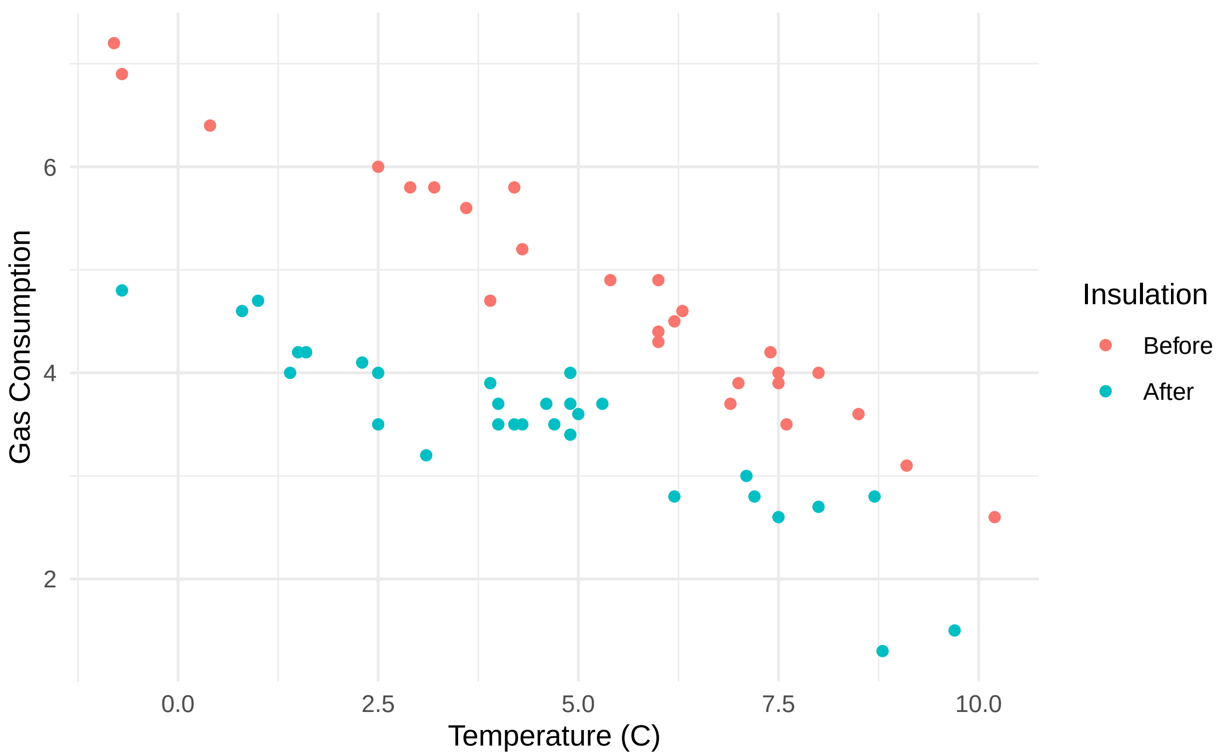
```
    fit   lwr   upr
1 6.854 6.151 7.557
2 4.888 4.227 5.548
3 2.921 2.228 3.614
4 4.724 4.034 5.414
5 3.334 2.675 3.994
6 1.945 1.238 2.651
```

Visualization of Confidence Intervals and Prediction Intervals

Example: Suppose we want to visualize the model for the `whiteside` data.

First consider a plot of the raw data.

```
p <- ggplot(MASS::whiteside, aes(x = Temp, y = Gas, color = Insul)) +
  geom_point() + theme_minimal() +
  labs(x = "Temperature (C)", y = "Gas Consumption", color = "Insulation")
plot(p)
```



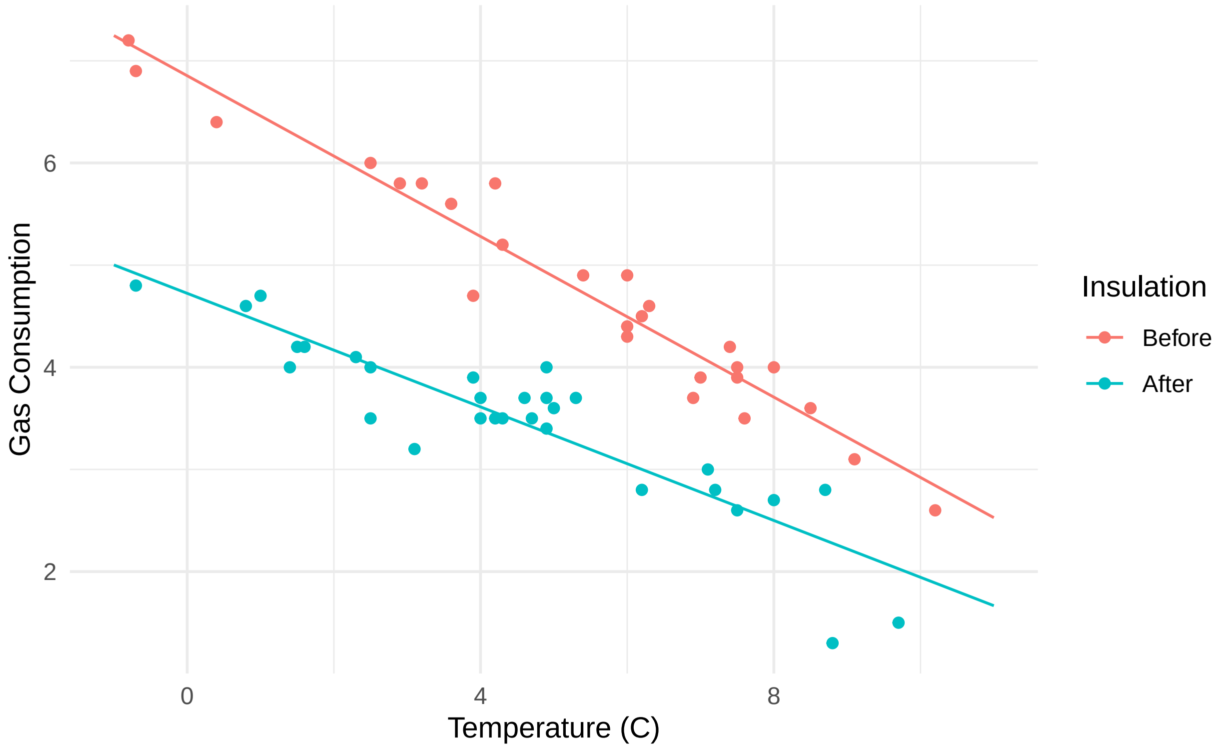
There are several ways we could show confidence intervals for the expected response or prediction intervals.

```
d <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, by = 1))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))
head(d)
```

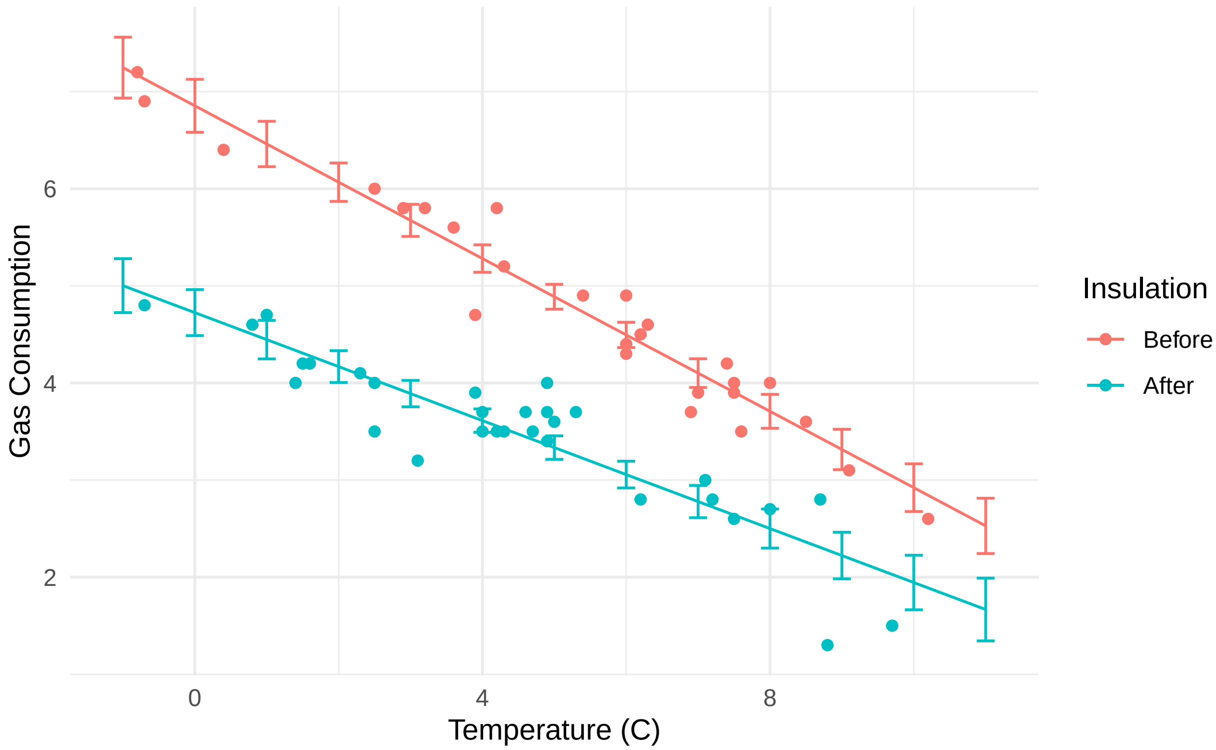
```
   Insul Temp   fit   lwr   upr
1 Before   -1 7.247 6.934 7.561
2  After   -1 5.002 4.724 5.280
```

```
3 Before     0 6.854 6.581 7.127
4  After     0 4.724 4.487 4.961
5 Before     1 6.461 6.227 6.694
6  After     1 4.446 4.247 4.644
```

```
p <- p + geom_line(aes(y = fit), data = d)
plot(p)
```

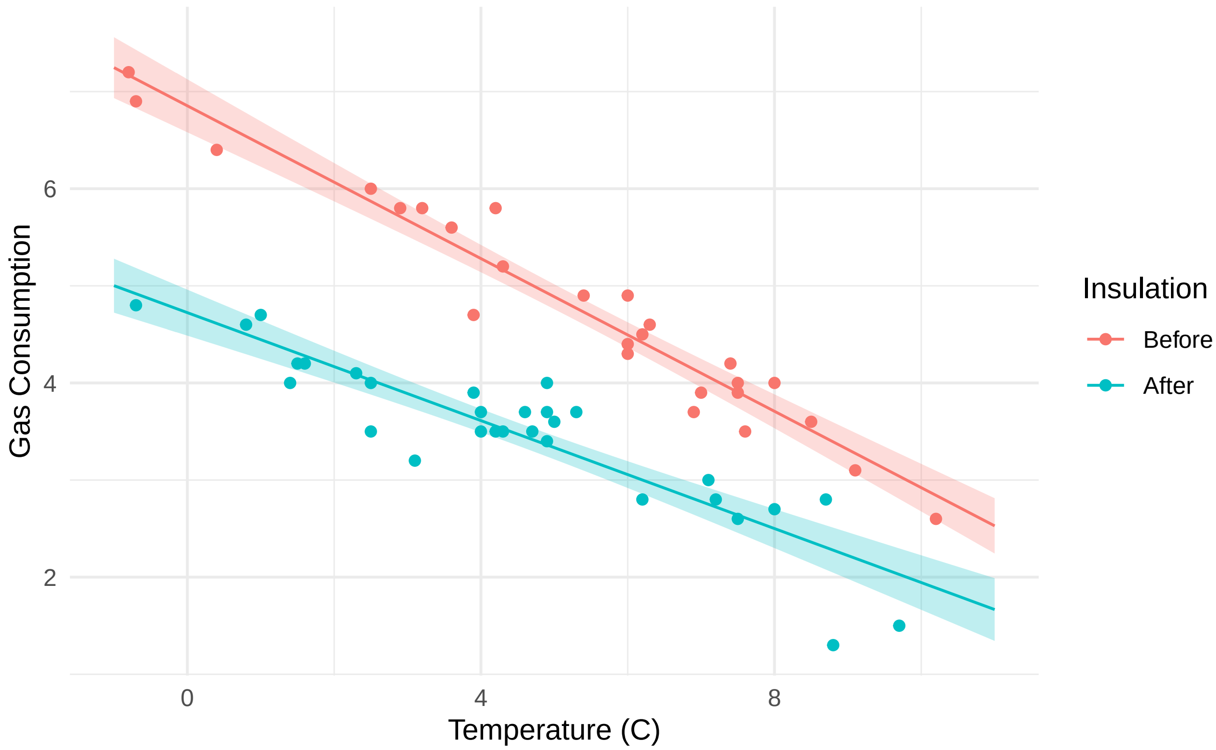



```
p <- p + geom_errorbar(aes(y = NULL, ymin = lwr, ymax = upr), width = 0.25, data = d)
plot(p)
```



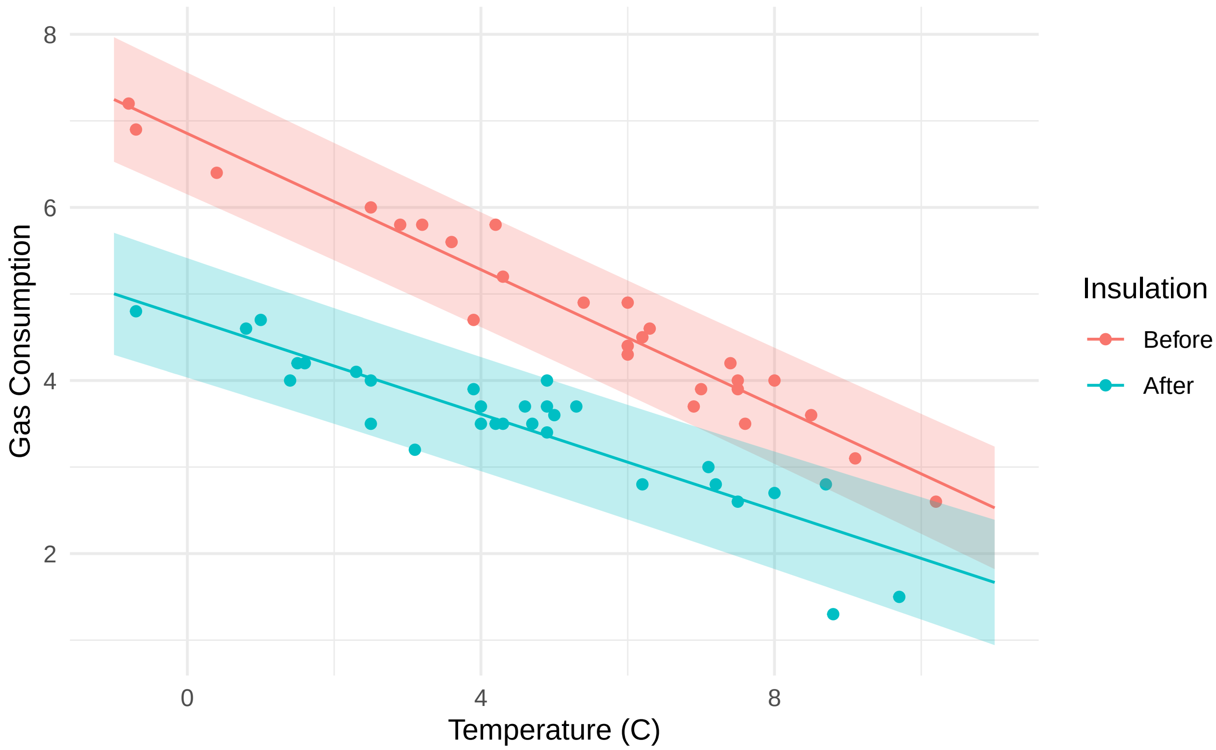
Here's another approach using confidence intervals for the expected response.

```
d <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))

p <- ggplot(MASS::whiteside, aes(x = Temp, y = Gas, color = Insul)) +
  geom_point() + theme_minimal() +
  labs(x = "Temperature (C)", y = "Gas Consumption", color = "Insulation") +
  geom_line(aes(y = fit), data = d) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr, fill = Insul),
    alpha = 0.25, color = NA, data = d, show.legend = FALSE)
plot(p)
```



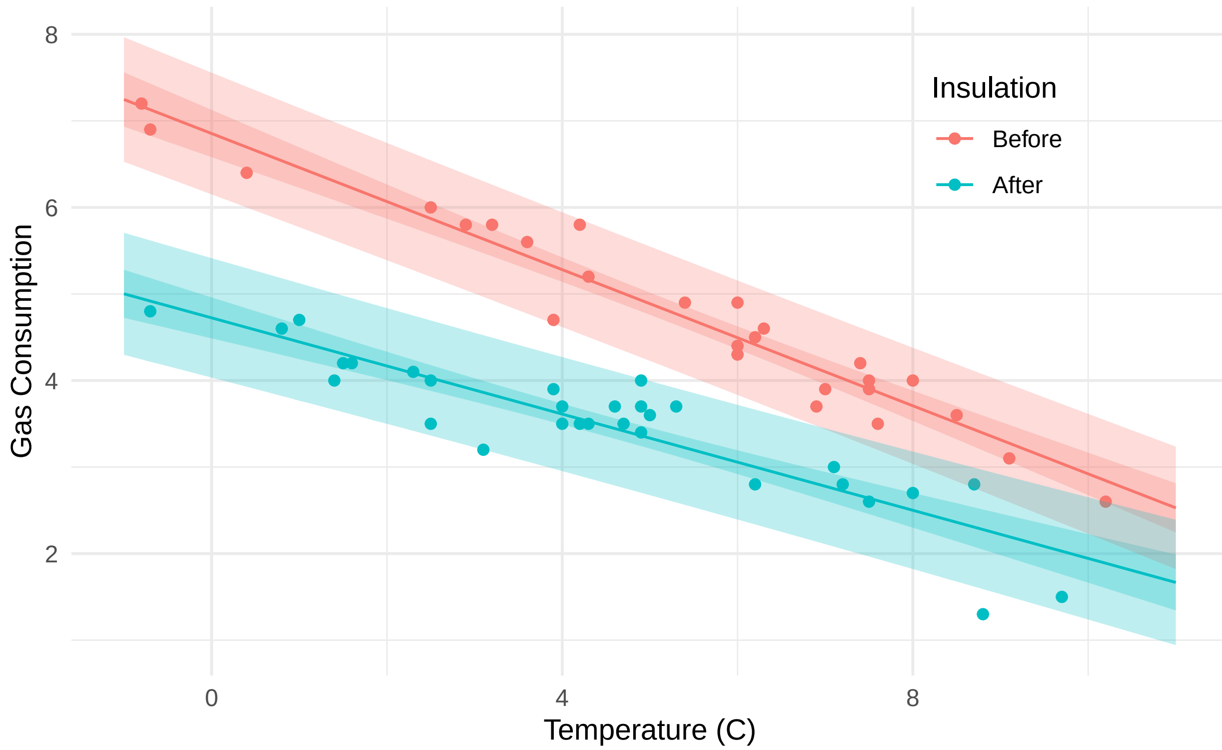
Same approach but now for prediction intervals.

```
d <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d <- cbind(d, predict(m, newdata = d, interval = "prediction"))

p <- ggplot(MASS::whiteside, aes(x = Temp, y = Gas, color = Insul)) +
  geom_point() + theme_minimal() +
  labs(x = "Temperature (C)", y = "Gas Consumption", color = "Insulation") +
  geom_line(aes(y = fit), data = d) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr, fill = Insul),
    alpha = 0.25, color = NA, data = d, show.legend = FALSE)
plot(p)
```



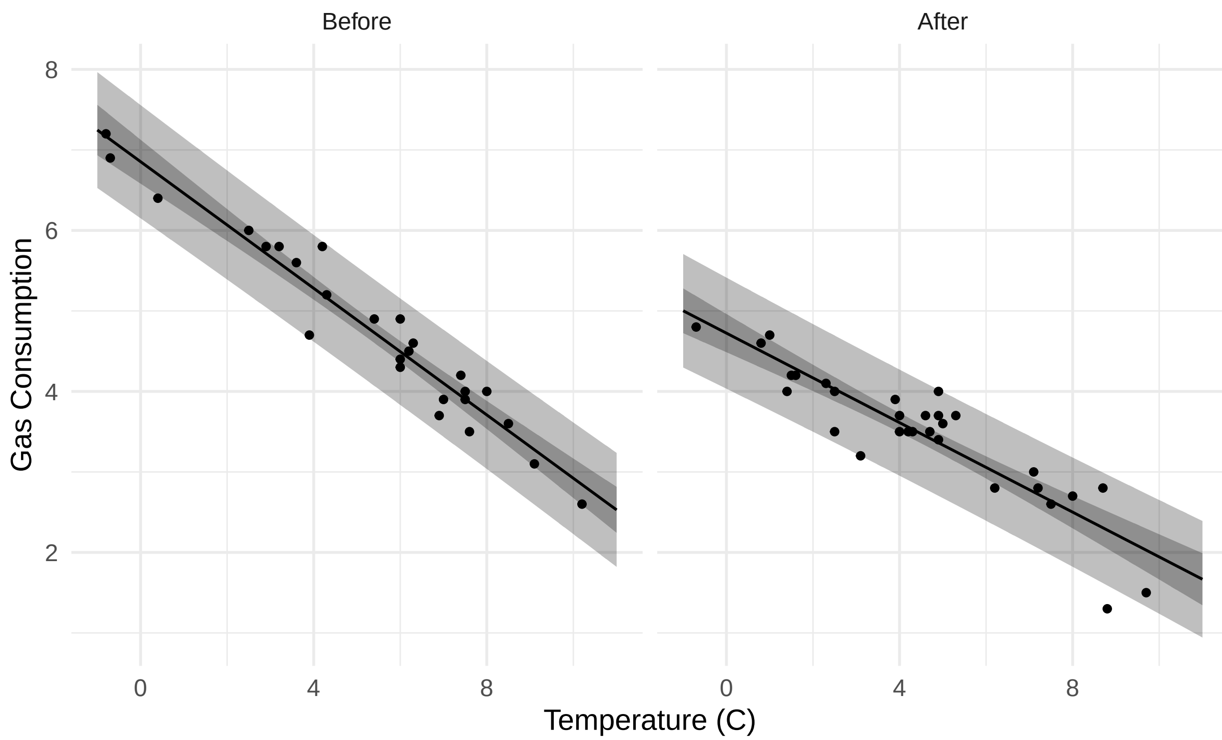
We can put them together, and move the legend.

```
d1 <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d1 <- cbind(d1, predict(m, newdata = d1, interval = "confidence"))

d2 <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d2 <- cbind(d2, predict(m, newdata = d2, interval = "prediction"))

p <- ggplot(MASS::whiteside, aes(x = Temp, y = Gas, color = Insul)) +
  geom_point() + theme_minimal() +
  labs(x = "Temperature (C)", y = "Gas Consumption", color = "Insulation") +
  geom_line(aes(y = fit), data = d1) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr, fill = Insul),
    alpha = 0.25, color = NA, data = d1, show.legend = FALSE) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr, fill = Insul),
    alpha = 0.25, color = NA, data = d2, show.legend = FALSE) +
  theme(legend.position = "inside", legend.position.inside = c(0.8,0.8))
plot(p)
```



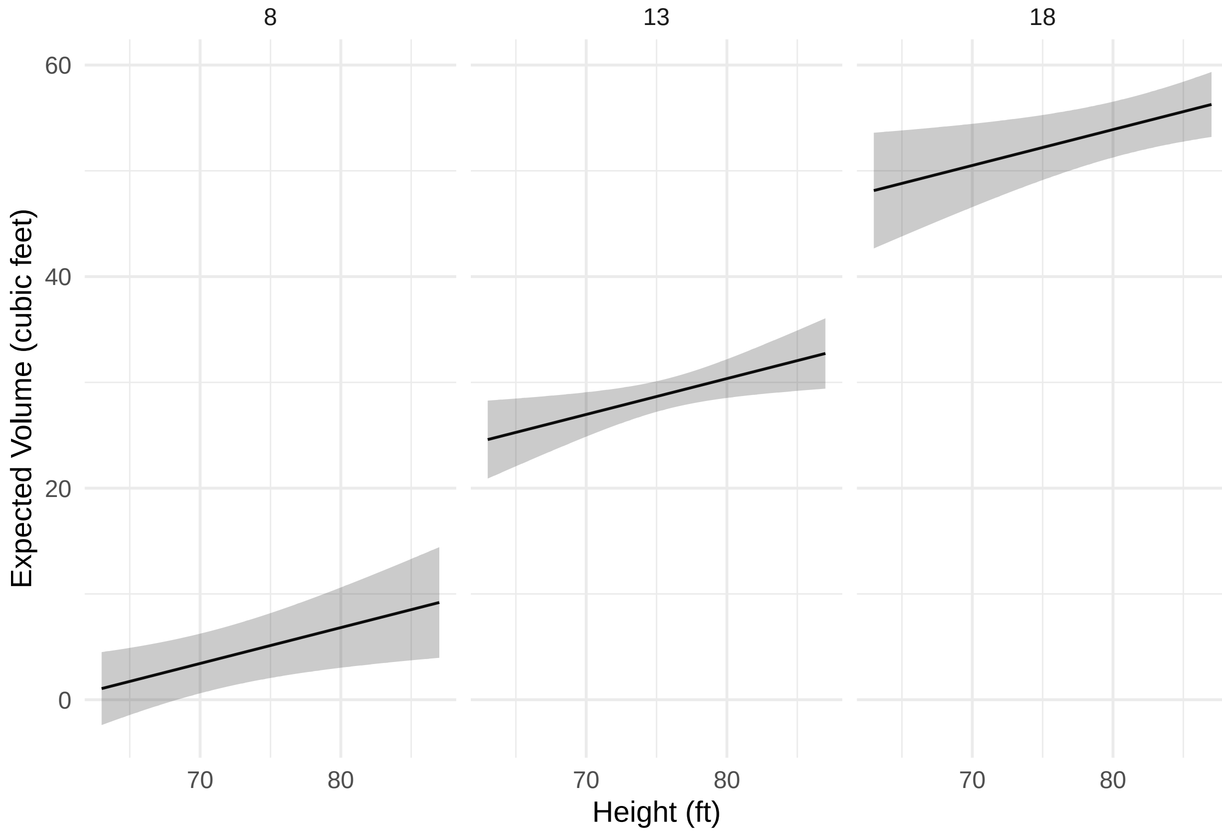
Black and white for the color printer challenged.

```
d1 <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d1 <- cbind(d1, predict(m, newdata = d1, interval = "confidence"))

d2 <- expand.grid(Insul = c("Before","After"), Temp = seq(-1, 11, length = 100))
d2 <- cbind(d2, predict(m, newdata = d2, interval = "prediction"))

p <- ggplot(MASS::whiteside, aes(x = Temp, y = Gas)) +
  geom_point(size = 1) + theme_minimal() + facet_wrap(~ Insul) +
  labs(x = "Temperature (C)", y = "Gas Consumption") +
  geom_line(aes(y = fit), data = d1) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr), fill = "black",
    alpha = 0.25, color = NA, data = d1, show.legend = FALSE) +
  geom_ribbon(aes(y = NULL, ymin = lwr, ymax = upr), fill = "black",
    alpha = 0.25, color = NA, data = d2, show.legend = FALSE)
plot(p)
```



Example: Consider visualizing several models for the `trees` data. How do we deal with having two quantitative explanatory variables?

```
m <- lm(Volume ~ Height + Girth, data = trees)

d <- expand.grid(Height = seq(63, 87, length = 100), Girth = c(8, 13, 18))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))

p <- ggplot(d, aes(x = Height, y = fit)) + theme_minimal() +
  geom_line() + facet_wrap(~ Girth) +
  geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.25) +
  labs(x = "Height (ft)", y = "Expected Volume (cubic feet)")
plot(p)
```



Now suppose there is a third categorical variable `Species`.

```
set.seed(123)
trees$Species <- sample(c("A","B"), 31, TRUE)
head(trees)
```

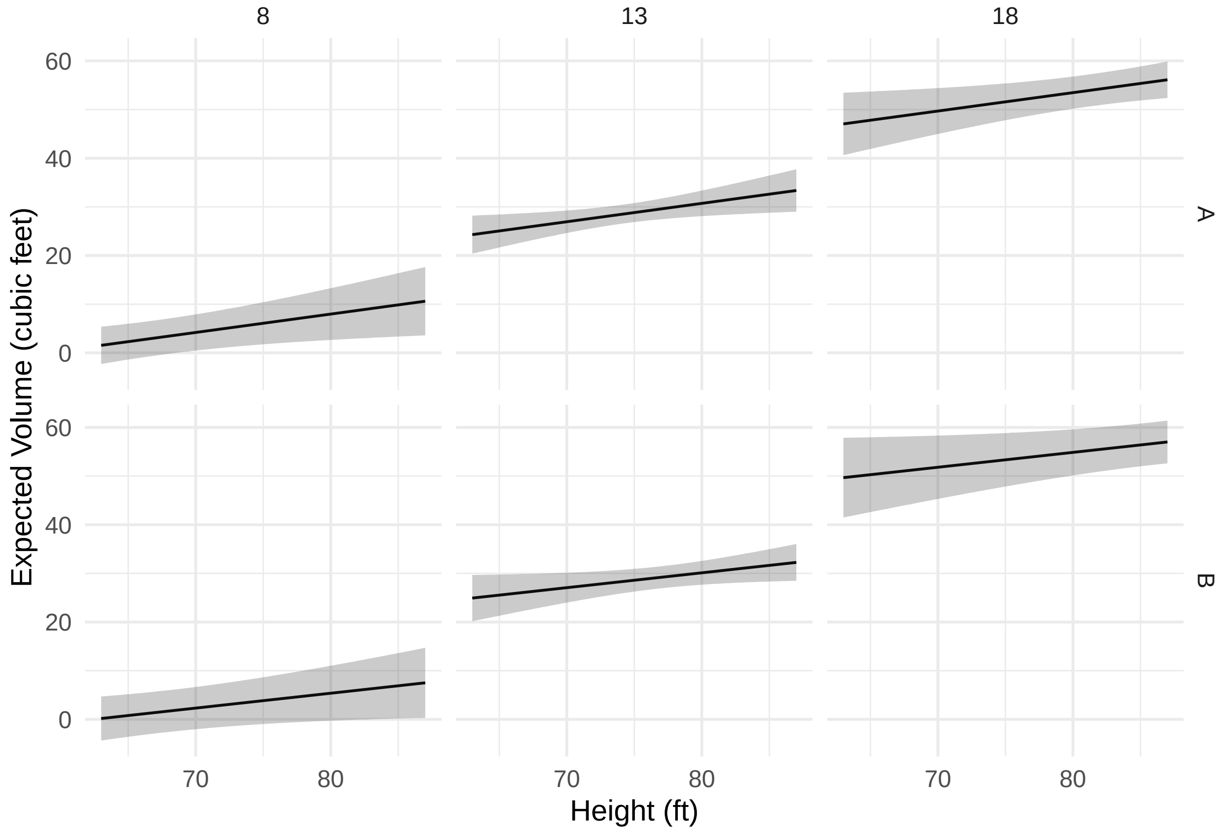
```
  Girth Height Volume Species
1   8.3     70   10.3       A
2   8.6     65   10.3       A
3   8.8     63   10.2       A
4  10.5     72   16.4       B
5  10.7     81   18.8       A
6  10.8     83   19.7       B
```

```
m <- lm(Volume ~ Height + Girth + Height:Species + Girth:Species, data = trees)
summary(m)$coefficients
```

```
                 Estimate Std. Error t value  Pr(>|t|)
(Intercept)     -58.67683    9.12536 -6.4301 8.195e-07
Height            0.37798    0.14777  2.5579 1.670e-02
Girth             4.55074    0.34654 13.1320 5.542e-13
Height:SpeciesB  -0.07239    0.09906 -0.7307 4.715e-01
Girth:SpeciesB    0.39908    0.56071  0.7117 4.830e-01
```

```
d <- expand.grid(Height = seq(63, 87, length = 100), Girth = c(8, 13, 18), Species = c("A","B"))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))

p <- ggplot(d, aes(x = Height, y = fit)) + theme_minimal() +
  geom_line() + facet_grid(Species ~ Girth) +
```

```
  geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.25) +
  labs(x = "Height (ft)", y = "Expected Volume (cubic feet)")
plot(p)
```



The help file for trees (see `?trees`) suggests the model

$$E(V_i) = \beta_1 h_i g_i^2,$$

which might be reasonable if we think of a tree as being approximately a cylinder or a cone and assume that expected volume is approximately proportional to the volume of a cylinder ($\pi(g/2)^2 h$ or $\pi g^2 h/4$) or cone ($\pi g^2 h/6$), noting that girth is diameter in this data set. Note that both volumes are *proportional to* $g^2 h$. So the expected volume could be written as

$$E(V_i) = \beta_0 + \beta_1 x_i,$$

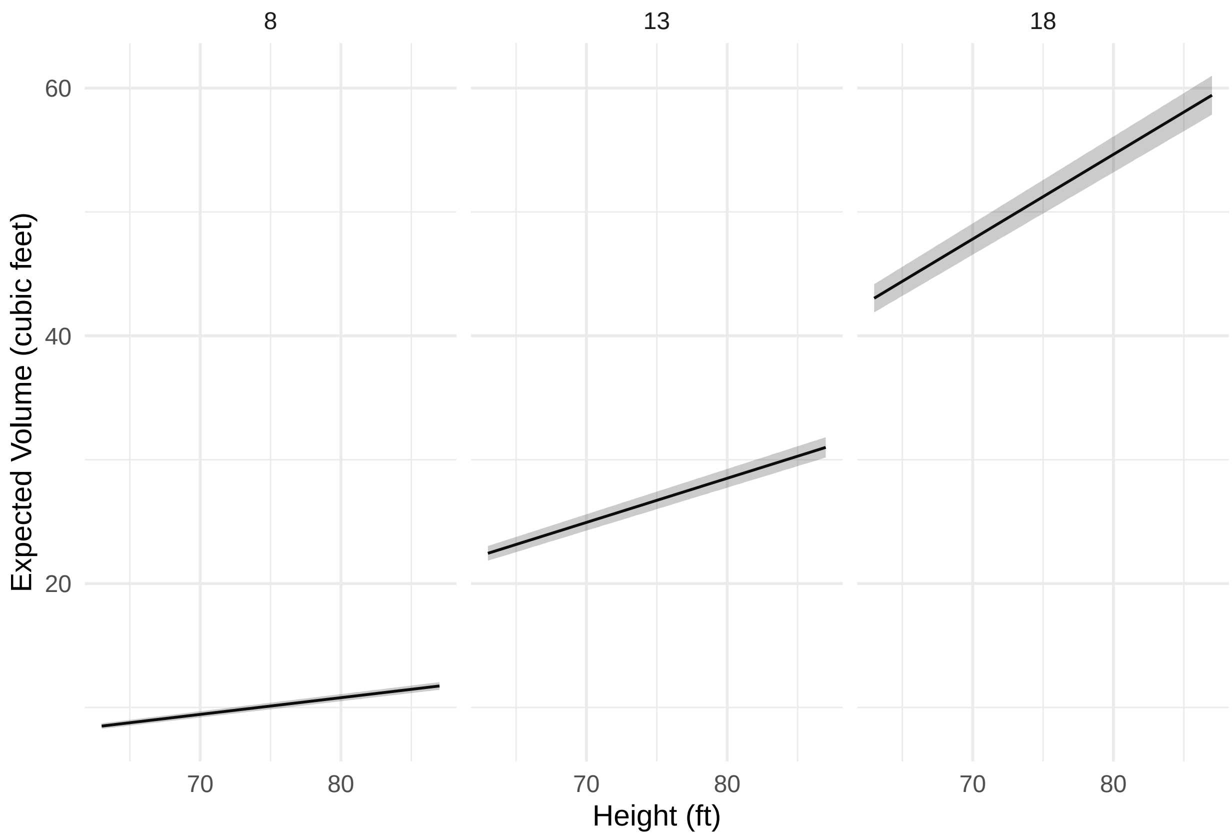
where $\beta_0 = 0$ and $x_i = h_i g_i^2$, where β_1 "absorbs" any constants in the volume calculation and also necessary due to the units used to measure these quantities. To specify $h_i g_i^2$ as an explanatory variable, we need to use `I()` to keep R from misinterpreting interpret '*' and '^' anything other than the mathematical operators.

```
m <- lm(Volume ~ -1 + I(Height*Girth^2), data = trees)
summary(m)$coefficients
```

```
                   Estimate Std. Error t value  Pr(>|t|)
I(Height * Girth^2) 0.002108  2.722e-05   77.44 4.137e-36
```

```
d <- expand.grid(Height = seq(63, 87, length = 100), Girth = c(8, 13, 18))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))

p <- ggplot(d, aes(x = Height, y = fit)) + theme_minimal() +
  geom_line() + facet_wrap(. ~ Girth) +
```

```r
  geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.25) +
  labs(x = "Height (ft)", y = "Expected Volume (cubic feet)")
plot(p)
```



Now suppose we specify the following model.

```r
m <- lm(Volume ~ -1 + I(Height*Girth^2):Species, data = trees)
summary(m)$coefficients
```

```
                          Estimate Std. Error t value  Pr(>|t|)
I(Height * Girth^2):SpeciesA 0.002094  3.505e-05   59.72 6.526e-32
I(Height * Girth^2):SpeciesB 0.002131  4.425e-05   48.17 3.132e-29
```

We can see that this model is

$$E(V_i) = \beta_1 h_i g_i^2 a_i + \beta_2 h_i g_i^2 b_i,$$

where

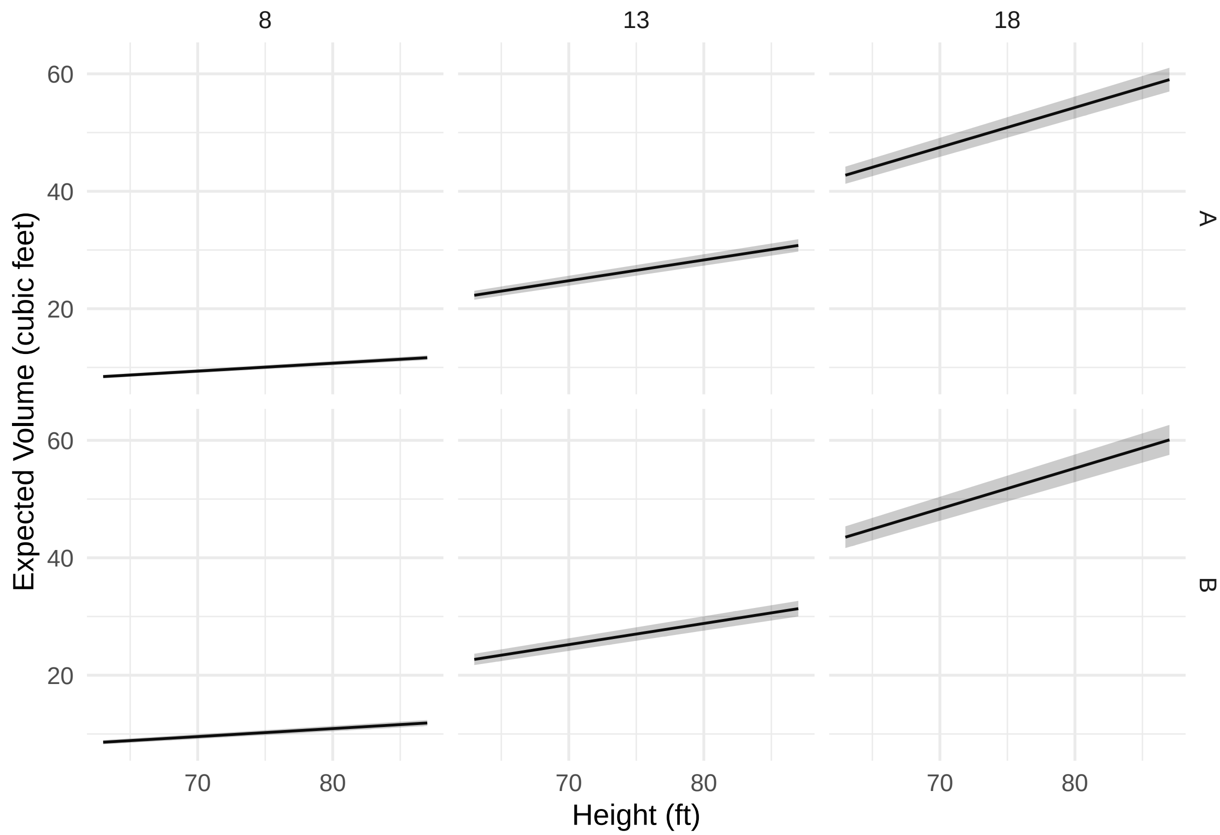
$$a_i = \begin{cases} 1, & \text{if the } i\text{-th observation is of species A,} \\ 0, & \text{otherwise,} \end{cases}$$

$$b_i = \begin{cases} 1, & \text{if the } i\text{-th observation is of species B,} \\ 0, & \text{otherwise,} \end{cases}$$

so we can write the model as

$$E(V_i) = \begin{cases} \beta_1 h_i g_i^2, & \text{if the } i\text{-th observation is of species A,} \\ \beta_2 h_i g_i^2, & \text{if the } i\text{-th observation is of species B.} \end{cases}$$

```r
d <- expand.grid(Height = seq(63, 87, length = 100),
  Girth = c(8, 13, 18), Species = c("A","B"))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))

p <- ggplot(d, aes(x = Height, y = fit)) + theme_minimal() +
  geom_line() + facet_grid(Species ~ Girth) +
  geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.25) +
  labs(x = "Height (ft)", y = "Expected Volume (cubic feet)")
plot(p)
```



Comparison of the two species:

```r
lincon(m, a = c(-1,1)) # b2 - b1
```

```
          estimate        se      lower     upper tvalue df pvalue
(-1,1),0 3.786e-05 5.645e-05 -7.759e-05 0.0001533 0.6707 29 0.5077
```

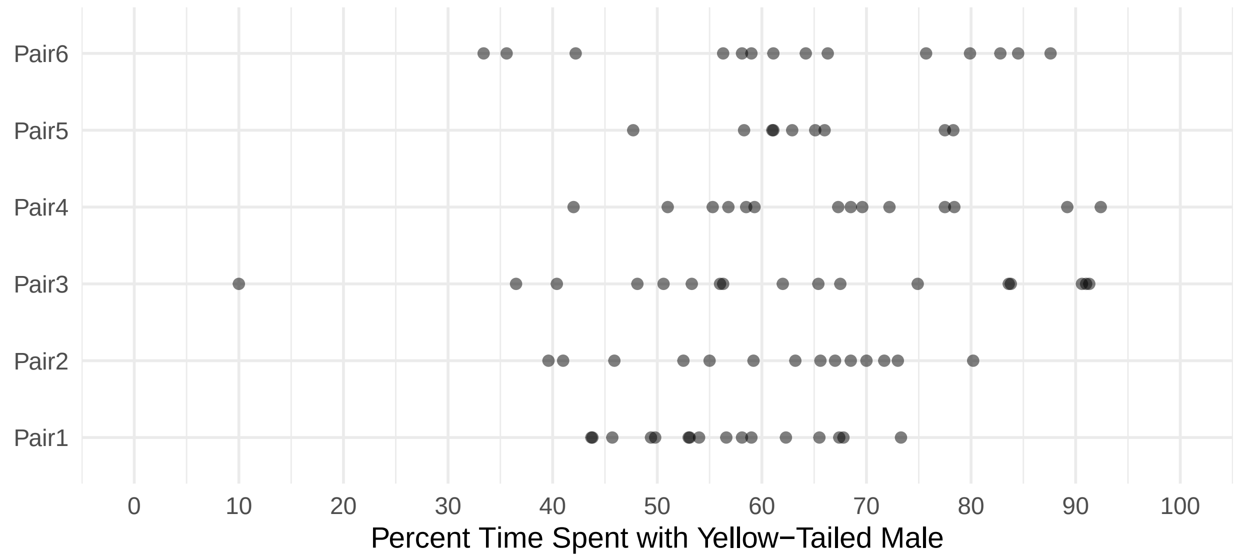
Example: Visualization of models for an experiment on mate preference in female platyfish.

Consider data from an experiment on mate preference in female platyfish.

```r
head(Sleuth3::case0602)
```

```
  Percentage  Pair Length
1       43.7 Pair1     35
2       54.0 Pair1     35
3       49.8 Pair1     35
4       65.5 Pair1     35
5       53.1 Pair1     35
6       53.0 Pair1     35
```

```r
p <- ggplot(Sleuth3::case0602, aes(x = Pair, y = Percentage)) +
  geom_point(alpha = 0.5) + theme_minimal() + coord_flip() +
  labs(x = NULL, y = "Percent Time Spent with Yellow-Tailed Male") +
  scale_y_continuous(breaks = seq(0, 100, by = 10), limits = c(0,100))
plot(p)
```



We will specify a model to allow for differences in the expected response over male pairs.

```r
m <- lm(Percentage ~ Pair, data = Sleuth3::case0602)
summary(m)$coefficients
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept)   56.406      3.864 14.5965 5.208e-24
PairPair2      4.479      5.657  0.7919 4.308e-01
PairPair3      6.023      5.384  1.1187 2.667e-01
PairPair4     10.594      5.657  1.8727 6.485e-02
PairPair5      7.805      6.441  1.2118 2.292e-01
PairPair6      6.929      5.657  1.2250 2.243e-01
```

Computing and plotting the estimated expected response for each pair.

```r
contrast(m, a = list(Pair = paste("Pair", 1:6, sep = "")),
  cnames = paste("Pair", 1:6, sep = ""))
```

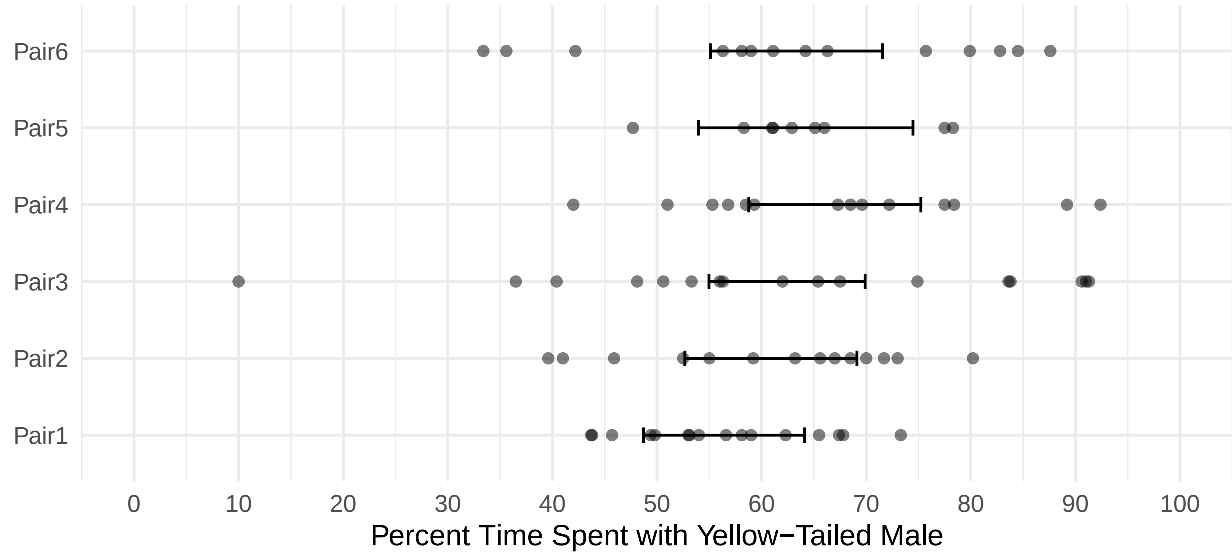
```
      estimate    se lower upper tvalue df    pvalue
Pair1    56.41 3.864 48.71 64.10  14.60 78 5.208e-24
Pair2    60.89 4.131 52.66 69.11  14.74 78 2.990e-24
Pair3    62.43 3.749 54.97 69.89  16.65 78 2.114e-27
Pair4    67.00 4.131 58.78 75.22  16.22 78 1.052e-26
Pair5    64.21 5.152 53.95 74.47  12.46 78 3.039e-20
Pair6    63.34 4.131 55.11 71.56  15.33 78 3.006e-25
```

```r
d <- data.frame(Pair = paste("Pair", 1:6, sep = ""))
d <- cbind(d, predict(m, newdata = d, interval = "confidence"))
d
```

```
   Pair   fit   lwr   upr
1 Pair1 56.41 48.71 64.10
2 Pair2 60.89 52.66 69.11
```

```
3 Pair3 62.43 54.97 69.89
4 Pair4 67.00 58.78 75.22
5 Pair5 64.21 53.95 74.47
6 Pair6 63.34 55.11 71.56
```

```
p <- p + geom_errorbar(aes(y = NULL, ymin = lwr, ymax = upr), width = 0.2, data = d)
plot(p)
```



Try replacing `confidence` with `prediction` to see prediction intervals.