Regression and ANOVA

Justin Patterson

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Contents

Preface

This project is meant to be a personal guide to ANOVA and regression. The scope of this project does not include time series analysis. Also, the focus will not be on designing experiments, but rather on analyzing the data from experiments which have already been conducted. To accomplish this, we will use simulated experimental data.

Disclaimer
This project was not written by an expert. That being said, I would appreciate any comments.

Note This book was constructed with the **bookdown** package [9], which was built on top of R Markdown and **knitr** [10].

Chapter 1

Introduction

You can label chapter and section titles using `{#label}` after them, e.g., we can reference Chapter 1. If you do not manually label them, there will be automatic labels anyway, e.g., Chapter 3.

Figures and tables with captions will be placed in `figure` and `table` environments, respectively.

```
par(mar = c(4, 4, .1, .1))
plot(pressure, type = 'b', pch = 19)
```

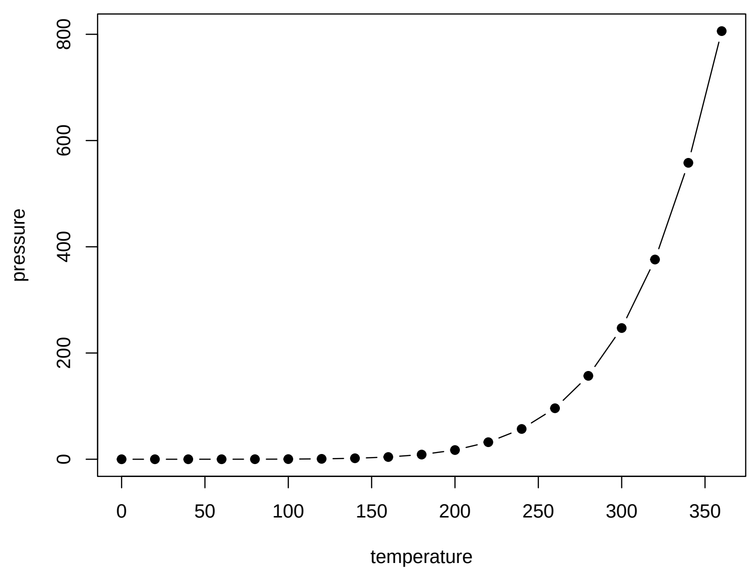


Figure 1.1: Here is a nice figure!

Table 1.1: Here is a nice table!

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
4.6	3.4	1.4	0.3	setosa
5.0	3.4	1.5	0.2	setosa
4.4	2.9	1.4	0.2	setosa
4.9	3.1	1.5	0.1	setosa
5.4	3.7	1.5	0.2	setosa
4.8	3.4	1.6	0.2	setosa
4.8	3.0	1.4	0.1	setosa
4.3	3.0	1.1	0.1	setosa
5.8	4.0	1.2	0.2	setosa
5.7	4.4	1.5	0.4	setosa
5.4	3.9	1.3	0.4	setosa
5.1	3.5	1.4	0.3	setosa
5.7	3.8	1.7	0.3	setosa
5.1	3.8	1.5	0.3	setosa

Reference a figure by its code chunk label with the `fig:` prefix, e.g., see Figure 1.1. Similarly, you can reference tables generated from `knitr::kable()`, e.g., see Table 1.1.

```
knitr::kable(
  head(iris, 20), caption = 'Here is a nice table!',
  booktabs = TRUE
)
```

Chapter 2

Literature

Here is a review of existing methods.

Chapter 3

Methods

We describe our methods in this chapter.

Chapter 4

Applications

Some *significant* applications are demonstrated in this chapter.

4.1 Example one

4.2 Example two

Chapter 5

Final Words

We have finished a nice book.

Chapter 6

ANOVA Fundamentals

Analysis of variance (ANOVA) is a collection of statistical models and their associated estimation procedures used to compare means. It may be difficult for the neophyte to understand, but ANOVA compares means by analyzing variances. ANOVA is based on the *Law of Total Variance* (6.1), where the observed variance in a particular variable is partitioned into components attributable to different sources of variation.[1]

6.1 Law of Total Variance

The law of total variance, also known as EVE's law [5][6], is very important for understanding how ANOVA works. The law says that for random variables X and Y on the same probability space, we have

$$\mathrm{Var}(Y) = \mathrm{E}[\mathrm{Var}(Y|X)] + \mathrm{Var}[\mathrm{E}(Y|X)]. \tag{6.1}$$

Let us consider the case of One-way ANOVA using Fixed Effects. We observe the random variable Y_{ij}, the j^{th} response for the i^{th} level of the single factor. Let A_i be the event where the i^{th} level of this factor is observed. Then 6.1 can be interpreted as

$$\mathrm{Var}(Y_{ij}) = \underbrace{\mathrm{E}[\mathrm{Var}(Y_{ij}|A_i)]}_{\substack{\text{variance of } Y \\ \text{within groups}}} + \underbrace{\mathrm{Var}[\mathrm{E}(Y_{ij}|A_i)]}_{\substack{\text{variance of } Y \\ \text{between groups}}} \tag{6.2}$$

Can 6.2 be simplified into something computationally useful for our ANOVA?

$$\mathrm{E}(Y_{ij}|A_i) = \sum_{j=1}^{n_i} y_{ij}\frac{1}{n_i} = \bar{y}_{i\cdot} \tag{6.3}$$

$$\mathrm{Var}(Y_{ij}|A_i) = \sum_{j=1}^{n_i} \left(y_{ij} - \bar{y}_{i\cdot}\right)^2 \frac{1}{n_i} \tag{6.4}$$

$$\sum_{i=1}^{k}\sum_{j=1}^{n_i} \left(y_{ij} - \bar{\bar{y}}\right)^2 \frac{1}{N} = \sum_{i=1}^{k} \left(\sum_{j=1}^{n_i} \left(y_{ij} - \bar{y}_{i\cdot}\right)^2 \frac{1}{n_i}\right) \frac{n_i}{N} + \sum_{i=1}^{k} \left(\bar{y}_{i\cdot} - \bar{\bar{y}}\right)^2 \frac{n_i}{N} \tag{6.5}$$

After multiplying both sides by N, we have this partition of the SS

$$\sum_{i=1}^{k}\sum_{j=1}^{n_i} \left(y_{ij} - \bar{\bar{y}}\right)^2 = \sum_{i=1}^{k}\sum_{j=1}^{n_i} \left(y_{ij} - \bar{y}_{i\cdot}\right)^2 + \sum_{i=1}^{k} n_i \left(\bar{y}_{i\cdot} - \bar{\bar{y}}\right)^2 \tag{6.6}$$

Recall [3] the definition of the mean of a population. Let X be a random variable with a finite number of finite outcomes

Recall [4][2] the definition of the expected value of a continuous random variable conditioned on an event.

Recall [8] that the population variance of a finite population of size N with values y_i and mean μ is

$$\sigma^2 = \frac{1}{N} \underbrace{\sum_{i=1}^{N} \left(y_i - \mu\right)^2}_{\text{SS}} \tag{6.7}$$

where the sum is known as a sum of squares (SS).

6.2 Partitioning the SS

```
source(file.path("src", "get-SS.R"))
```

Let's look at this simulated experiment to see the SS Decomposition in action. How can we explain the variation that we see in the response?

```
source(file.path("src", "partitioning-SS.R"))
```

```
##
## Attaching package: 'dplyr'
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

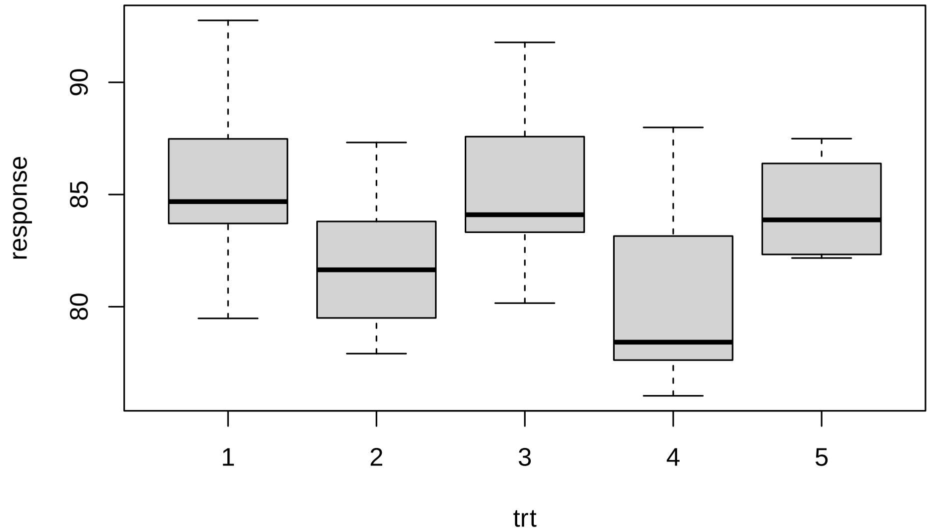


Figure 6.1: Responses were simulated for five different levels of a single factor. The respective sample sizes for each treatment group were 10, 14, 13, 9, and 8.

$$SS_{\text{total}} = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \left(y_{ij} - \bar{\bar{y}}\right)^2 = 739.971$$

$$SS_{\text{within}} = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \left(y_{ij} - \bar{y}_{i\cdot}\right)^2 = 558.06$$

$$SS_{\text{between}} = \sum_{i=1}^{k} n_i \left(\bar{y}_{i\cdot} - \bar{\bar{y}}\right)^2 = 181.911$$

Notice that $SS_{\text{total}} = SS_{\text{within}} + SS_{\text{between}}$. Also, $\frac{SS_{\text{total}}}{n-1} = s^2 = 13.962$.

```
summary(aov(response ~ trt, data = fabricated_data))
```

```
##             Df Sum Sq Mean Sq F value  Pr(>F)
## trt          4  181.9   45.48   3.993 0.00699 **
## Residuals   49  558.1   11.39
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
library(cellWise)
library(knitr)
opts_chunk$set(tidy.opts=list(width.cutoff=50),tidy=TRUE)
```

6.3 Step 1: Make up Data

```
# dataset1
```

6.4 Checking the Assumptions

After running your ANOVA, check that the assumptions about the errors are met so that you can do statistical inference. Those assumptions are:

1. $\mathrm{E}(\epsilon_{ij}) = 0,\ \mathrm{Var}(\epsilon_{ij}) = \sigma_i^2 < \infty,$ for all i, j.
2. The ϵ_{ij} are mutually independent and normally distributed.
3. $\sigma_i^2 = \sigma^2$ for all i.

6.4.1 Checking Assumption 1

6.4.2 Assumption 1 was violated.

6.4.3 Checking Assumption 2

6.4.4 Assumption 2 was violated.

6.4.5 Checking Assumption 3

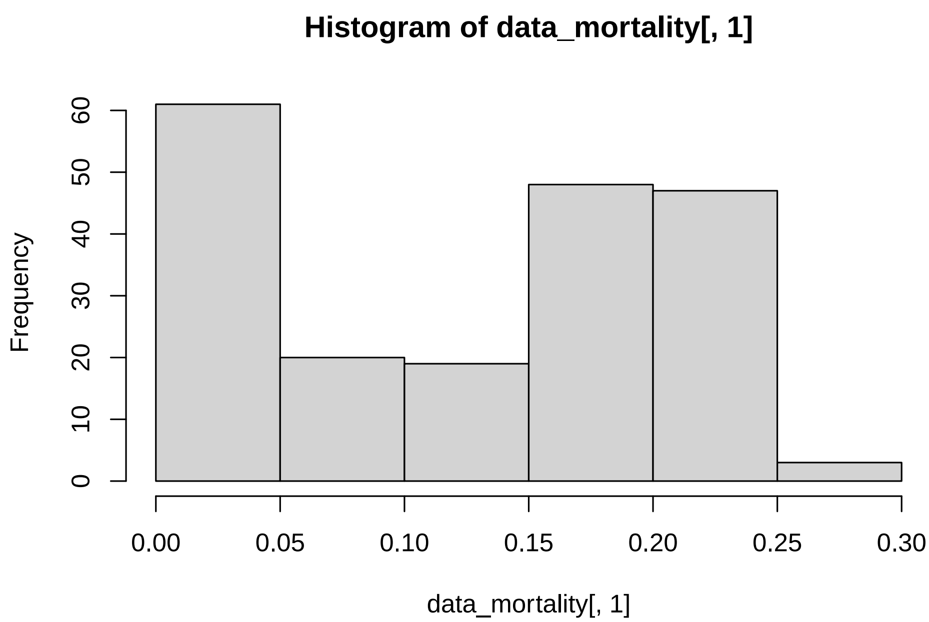
6.4.6 Assumption 3 was violated.

A variance-stabilizing transformation of the response variable may help.

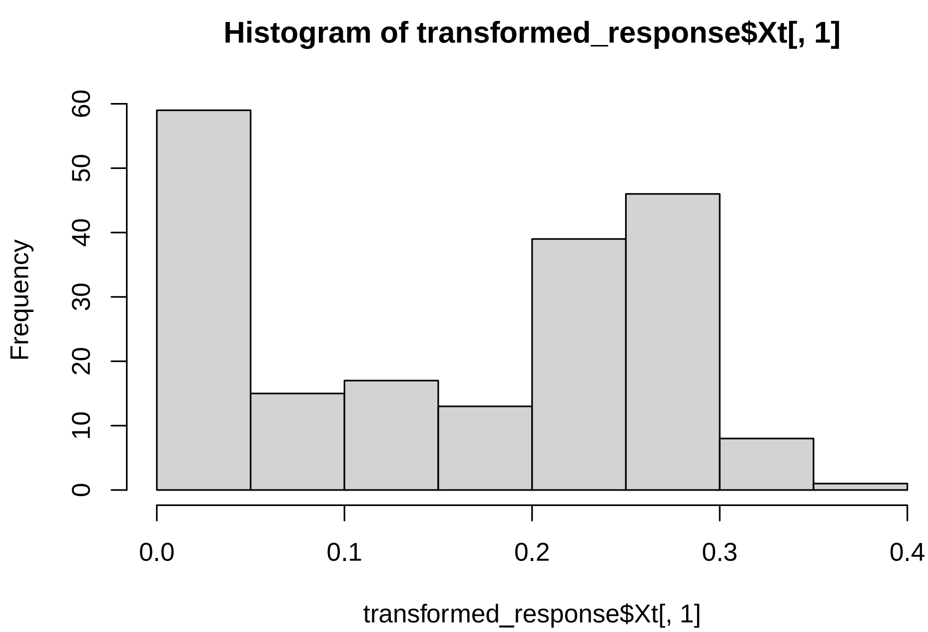
```
data("data_mortality")
transformed_response = transfo(data_mortality, prestandardize = FALSE)
```

```
##
##  The input data has 198 rows and 91 columns.
```

```
hist(data_mortality[, 1])
```




```
hist(transformed_response$Xt[, 1])
```



```
shapiro.test(data_mortality[, 1])
```

```
##
##  Shapiro-Wilk normality test
##
## data:  data_mortality[, 1]
## W = 0.86877, p-value = 4.552e-12
```

```
shapiro.test(transformed_response$Xt[, 1])
```

```
##
##  Shapiro-Wilk normality test
##
## data:  transformed_response$Xt[, 1]
## W = 0.88041, p-value = 1.968e-11
```

6.5 Regression and Categorical Variables

```
library(tidymodels)
```

```
## Registered S3 method overwritten by 'tune':
##   method                   from
##   required_pkgs.model_spec parsnip
```

```
## -- Attaching packages -------------------------------------- tidymodels 0.1.3 --
```

```
## v broom        0.7.6      v rsample      0.1.0
## v dials        0.0.9      v tibble       3.1.2
## v ggplot2      3.3.3      v tidyr        1.1.3
## v infer        0.5.4      v tune         0.1.5
## v modeldata    0.1.0      v workflows    0.2.2
## v parsnip      0.1.6      v workflowsets 0.0.2
## v purrr        0.3.4      v yardstick    0.0.8
## v recipes      0.1.16
```

```
## -- Conflicts ----------------------------------------- tidymodels_conflicts() --
## x purrr::discard() masks scales::discard()
## x dplyr::filter()  masks stats::filter()
## x dplyr::lag()     masks stats::lag()
## x recipes::step()  masks stats::step()
## * Use tidymodels_prefer() to resolve common conflicts.
```

```
library(ggplot2)
```

There is a profound connection between linear regression and ANOVA. In order to see this, you have to understand that the categorical variables of an ANOVA can be coded with numbers, which allows them to be used in a linear regression model. Let us recall [7] the multiple linear regression model.

Given a random sample of n observations $(Y_i, X_{i1}, ..., X_{ip}),\ i = 1, ..., n$, the basic multiple linear regression model is

$$Y_i = \beta_0 + \beta_1 X_{i1} + ... + \beta_p X_{ip} + \epsilon_i, \quad i = 1, ..., n$$

where each ϵ_i is a random variable with a mean of 0. In matrix form, this can be written as

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{1,1} & X_{1,2} & \dots & X_{1,p} \\ 1 & X_{2,1} & X_{2,2} & \dots & X_{2,p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & X_{n,1} & X_{n,2} & \dots & X_{n,p} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_0 \\ \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Here, the $X_{i,j}$ represent our coded categorical variables. These categorical variables are coded according to the hypotheses of interest. In many cases, the coding is done so that the newly coded variables are contrasts of the old categorical variables.

A contrast is a linear combination of variables such that the coefficients sum to 0.

$$\sum_i a_i \theta_i \quad \text{such that} \quad \sum_i a_i = 0$$

Unlike in ANOVA, in regression, it is best to use coding schemes based on orthogonal and fractional contrasts. Orthogonal contrasts are a set of contrasts in which, for any distinct pair, the sum of the cross-products of the coefficients is 0.

$$\sum_i a_i b_i = 0$$

I believe that a fractional contrast is such that

$$\sum_i |a_i| = 2$$

Categorical variable coding schemes can be easily expressed in a matrix format. The convention is to have the old categorical variables as the row headers and the newly coded variables as the column headers. In such a matrix, the $[c_{ij}]$ entry indicates the value of the j^{th} level of the new variable for the i^{th} level of the old variable. Here is an example of such a matrix constructed using orthogonal and fractional contrasts.

```
(contr_mat = matrix(data = c(1, 0, -1, 0.5, -1, 0.5),
    nrow = 3, ncol = 2))
```

```
##      [,1] [,2]
## [1,]    1  0.5
## [2,]    0 -1.0
## [3,]   -1  0.5
```

Interpreting this coding scheme in the context of our linear model, we see that

$$
\begin{aligned}
E(Y_i|X_{i1}=1, X_{i2}=\tfrac{1}{2}) &= \beta_0+\beta_1+\tfrac{1}{2}\beta_2 &= \mu_1 \\
E(Y_i|X_{i1}=0, X_{i2}=-1) &= \beta_0-\beta_2 &= \mu_2 \\
E(Y_i|X_{i1}=-1, X_{i2}=\tfrac{1}{2}) &= \beta_0-\beta_1+\tfrac{1}{2}\beta_2 &= \mu_3
\end{aligned}
$$

or, in matrix format,

$$
\begin{bmatrix} 1 & 1 & \frac{1}{2} \\ 1 & 0 & -1 \\ 1 & -1 & \frac{1}{2} \end{bmatrix}
\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}
=
\begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix}
$$

We can solve this for β for interpretation's sake.

```
solve(cbind(rep(1, nrow(contr_mat)), contr_mat))
```

```
##           [,1]       [,2]       [,3]
## [1,] 0.3333333  0.3333333  0.3333333
## [2,] 0.5000000  0.0000000 -0.5000000
## [3,] 0.3333333 -0.6666667  0.3333333
```

$$
\begin{aligned}
\beta_0 = && \tfrac{\mu_1+\mu_2+\mu_3}{3} && = && \text{grand mean response} \\
2\beta_1 = && \mu_1-\mu_3 && = && \text{difference in the mean response between levels 1 and 3 of the old categorical variable} \\
\tfrac{3}{2}\beta_2 = && \tfrac{\mu_1+\mu_3}{2}-\mu_2 && = && \text{difference in the mean response between level 2 and the average of levels 1 and 3 of the old categorical variable}
\end{aligned}
$$

Let's look at another contrast matrix and see if we can interpret it.

```
contr.helmert(n = 3)
```

```
##   [,1] [,2]
## 1   -1   -1
## 2    1   -1
## 3    0    2
```

```
solve(cbind(rep(1, 3), contr.helmert(n = 3)))
```

```
##               1          2         3
## [1,]  0.3333333  0.3333333 0.3333333
## [2,] -0.5000000  0.5000000 0.0000000
## [3,] -0.1666667 -0.1666667 0.3333333
```

$\beta_0 =$	$\frac{\mu_1+\mu_2+\mu_3}{3}$	$=$	grand mean response
$2\beta_1 =$	$\mu_2 - \mu_1$	$=$	difference in the mean response between levels 2 & 1 of the old categorical variable
$3\beta_2 =$	$\mu_3 - \frac{\mu_1+\mu_2}{2}$	$=$	difference in the mean response between level 3 and the average of levels 1 and 2 of the old categorical variable

Perhaps you have heard of polynomial regression? Polynomial regression is just a special case of linear regression in a different basis. In polynomial regression, (just like multiple linear regression) if you use all of your explanatory variables, then you will likely get multi-collinearity problems.

```
contr.poly(n = 3)
```

```
##                  .L         .Q
## [1,] -7.071068e-01  0.4082483
## [2,] -7.850462e-17 -0.8164966
## [3,]  7.071068e-01  0.4082483
```

```
(A = solve(cbind(rep(1, 3), contr.poly(n = 3))))
```

```
##           [,1]       [,2]      [,3]
##      0.3333333  0.3333333 0.3333333
## .L -0.7071068  0.0000000 0.7071068
## .Q  0.4082483 -0.8164966 0.4082483
```

The first matrix shows how to code the levels of your categorical variable and the second matrix is used for interpretation.

$\beta_0 =$	$\frac{\mu_1+\mu_2+\mu_3}{3}$	$=$	grand mean response
$\beta_1 =$	$-0.707\mu_1 + 0.707\mu_3$	$=$	measure of a linear trend in the mean response
$\beta_2 =$	$0.408\mu_3 - 0.816\mu_2 + 0.408\mu_3$	$=$	measure of a quadratic trend in the mean response

For example, we can test whether the difference between the means from two populations are equal by doing a linear regression or an ANOVA.

Let's make up some data and try it!

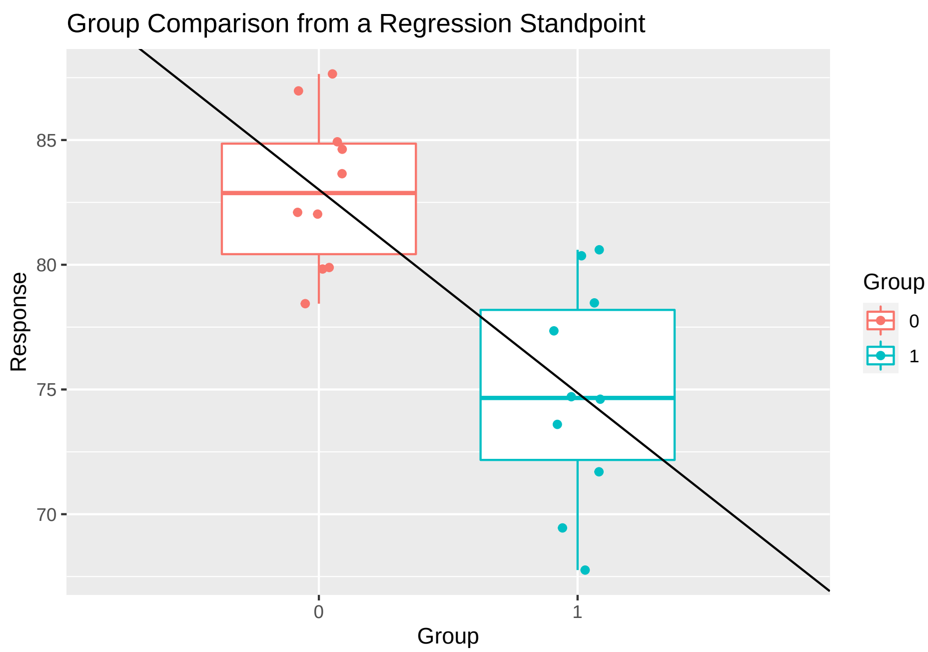
```
source(file.path("src", "fabricate.R"))
design = data.frame(group = c(0, 1), n = c(10, 10))
data1 = fabricate(flr = design)
```

Let's check out our data.

```
# Make a linear model
data1_lm_independent_samples = lm(response ~ group,
    data = data1)
# plot
ggplot(data = data1, aes(x = group, y = response, color = factor(group))) +
```

```
  geom_boxplot() + geom_jitter(height = 0, width = 0.1) +
  geom_abline(intercept = data1_lm_independent_samples$coefficients[1],
      slope = data1_lm_independent_samples$coefficients[2]) +
  labs(title = "Group Comparison from a Regression Standpoint",
      color = "Group", x = "Group", y = "Response") +
  scale_x_discrete(limits = c(0, 1))
```

```
## Warning: Continuous limits supplied to discrete scale.
## Did you mean `limits = factor(...)` or `scale_*_continuous()`?
```



The way you code your categorical variables in a linear model is extremely important. Different codings lead to different interpretations of the parameters (betas) in your model. For us, our model is

$$Y_i = \beta_0 + \beta_{i1} X_{i1} + \epsilon_i$$

From this, we have

$$E(Y_i | X_{i1} = 0) = \beta_0$$
$$E(Y_i | X_{i1} = 1) = \beta_0 + \beta_1$$

From which we can derive,

$$\beta_1 = E(Y_i | X_{i1} = 1) - E(Y_i | X_{i1} = 0)$$

So, our slope estimate is the estimated amount by which the mean of group1 is above that of the mean of group0.

Run linear regression

```
summary(data1_lm_independent_samples)
```

```
##
## Call:
## lm(formula = response ~ group, data = data1)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -7.101 -3.132 -0.201  2.769  5.739
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   83.012      1.202  69.041  < 2e-16 ***
## group         -8.151      1.700  -4.794 0.000145 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.802 on 18 degrees of freedom
## Multiple R-squared:  0.5607, Adjusted R-squared:  0.5363
## F-statistic: 22.98 on 1 and 18 DF,  p-value: 0.0001454
```

Run ANOVA

```
data1$group = as.factor(data1$group)
data1_ANOVA_independent_samples = aov(response ~ group,
    data = data1)
summary(data1_ANOVA_independent_samples)
```

```
##             Df Sum Sq Mean Sq F value   Pr(>F)
## group        1  332.2   332.2   22.98 0.000145 ***
## Residuals   18  260.2    14.5
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Run t-Test

```
(data1_t_test_independent_samples = t.test(x = data1[data1$group ==
    1, "response"], y = data1[data1$group == 0, "response"],
    paired = FALSE, var.equal = TRUE))
```

```
##
##  Two Sample t-test
##
## data:  data1[data1$group == 1, "response"] and data1[data1$group == 0, "response"]
```

```
## t = -4.7936, df = 18, p-value = 0.0001454
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  -11.723377  -4.578623
## sample estimates:
## mean of x mean of y
##    74.861    83.012
```

Notice the similarities.

```
# Confidence interval for the difference in the
# means
confint(data1_lm_independent_samples, "group", level = 0.95)
```

```
##           2.5 %    97.5 %
## group -11.72338 -4.578623
```

```
data1_t_test_independent_samples$conf.int
```

```
## [1] -11.723377  -4.578623
## attr(,"conf.level")
## [1] 0.95
```

```
# p-values
with(summary(data1_lm_independent_samples), unname(pf(fstatistic[1],
    fstatistic[2], fstatistic[3], lower.tail = F)))
```

```
## [1] 0.0001454089
```

```
summary(data1_ANOVA_independent_samples)[[1]][[1, 5]]
```

```
## [1] 0.0001454089
```

```
data1_t_test_independent_samples$p.value
```

```
## [1] 0.0001454089
```

Now, let's look at something else. The CO2 data frame has 84 rows and 5 columns of data from an experiment on the cold tolerance of the grass species Echinochloa crus-galli.

```
data("CO2")
CO2[sample(nrow(CO2), size = 5), ]
```

```
##    Plant        Type  Treatment conc uptake
## 41   Qc3      Quebec    chilled  675   39.6
## 6    Qn1      Quebec nonchilled  675   39.2
## 83   Mc3 Mississippi    chilled  675   18.9
## 37   Qc3      Quebec    chilled  175   21.0
## 73   Mc2 Mississippi    chilled  250   12.3
```

What is a linear model? In the context of linear regression, a linear model is a relationship between the responses and the explanatory variables that is linear in the parameters.

```
CO2_recipe = recipe(uptake ~ ., data = CO2) %>%
    step_dummy(c("Type", "Treatment"))
# see contrasts() function
CO2_linear_model = linear_reg() %>%
    set_engine("lm", contrasts = list(Plant = "contr.poly"))
CO2_workflow = workflow() %>%
    add_model(CO2_linear_model) %>%
    add_recipe(CO2_recipe)
CO2_fit = CO2_workflow %>%
    fit(data = CO2)
```

```
CO2_fit %>%
    pull_workflow_fit() %>%
    tidy()
```

```
## # A tibble: 15 x 5
##    term              estimate std.error statistic   p.value
##    <chr>                <dbl>     <dbl>     <dbl>     <dbl>
##  1 (Intercept)        19.5      1.17       16.7    2.96e-26
##  2 Plant.L           -22.9      2.27      -10.1    2.17e-15
##  3 Plant.Q            -4.62     2.27       -2.03   4.57e- 2
##  4 Plant.C             4.67     2.27        2.06   4.34e- 2
##  5 Plant^4             2.34     2.27        1.03   3.06e- 1
##  6 Plant^5             4.31     2.27        1.90   6.13e- 2
##  7 Plant^6            -0.0390   2.27       -0.0172 9.86e- 1
##  8 Plant^7            -2.04     2.27       -0.897  3.73e- 1
##  9 Plant^8            -3.28     2.27       -1.44   1.53e- 1
## 10 Plant^9            -9.07     2.27       -4.00   1.56e- 4
## 11 Plant^10            0.546    2.27        0.241  8.10e- 1
## 12 Plant^11            1.91     2.27        0.843  4.02e- 1
## 13 conc                0.0177   0.00223     7.96   1.97e-11
## 14 Type_Mississippi   NA       NA          NA      NA
## 15 Treatment_chilled  NA       NA          NA      NA
```

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