

# An Incomplete Solutions Guide to the NIST/SEMATECH e-Handbook of Statistical Methods

examples and case studies using the tidyverse and ggplot2

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# Preface

Exploratory Data Analysis (EDA) is a philosophy on how to work with data, and for many applications, the workflow is better suited for most working scientist and engineers. As a scientist, we are trained to formulate a hypothesis and design a series of experiments that will allow us to test the hypothesis effectively. Unfortunately, most data doesn't come from carefully controlled trials, but from observations. Statisticians will readily jump into describing the difference in as much detail as you would like.

For most of us, we need tools to characterize an instrument or a process. The philosophy of EDA provides the framework to do this work.

Unfortunately, most textbooks still focus on traditional statistical techniques and even while it is essential to understand the underlying assumptions and fundamentals, I would argue that most of the work we do as scientist and engineers are not well suited for rigorous statistical analysis. In many cases, the need to disseminate information to a broad audience is best served by the methods espoused by EDA. The NIST e-Handbook Engineering Statistics is a welcome deviation from the norm.

In the Spring of 2018, I adopted this text as the basis of a one-semester, graduate course that focused applied statistical techniques. The audience for this course were working scientist, and the course was a core course in a Professional Science Master's (PSM).

Unfortunately, the one drawback of the NIST Handbook is the use of Dataplot as the primary software package for analysis. The authors have provided examples using the R statistical language; however, most—if not all—of these scripts are written using base R which is unfortunate. Modern R now incorporates many packages for streamlining the EDA process. This book attempts to capture my efforts to use these methods and share them with students in the course. The two packages that I primarily used were **tidyverse** and **ggplot2**.

Before going further, I should clarify one thing—I'm a hack. I classify learning as three levels: novice, hack, expert.

Novice: basic knowledge of how to use a tool with a desire to learn. Hack: Basic to intermediate knowledge of how to use a tool accompanied by resources to produce a finished product. Expert: Extensive knowledge of how to use a tool; can produce a finished product with few outside resources.

I'm sure other factors can be added to each category, but these capture the spirit of how I approach learning.

The number of resources available to learn R is numerous, and the first I would strongly recommend is R for Data Science. This text is an introduction to the tidyverse. The tidyverse is not just a collection of R packages, but a philosophy on how to work with data. It makes data analysis almost fun!

The other primary resource available for EDA is ggplot2. Like the tidyverse, ggplot2 is not just a package of tools, but a philosophy built around the Grammar of Graphics.

I encourage the reader to explore the references related to these two packages and their underlying design philosophies.

This book will show how I have worked through the exercises and case studies presented in the NIST handbook using methods found in the tidyverse and ggplot2. I have found this framework to be incredibly

satisfying and one I was eager to share beyond my class.

If you find this material useful, please send me an email.

## Structure of the book

Content was built around the e-book NIST/SEMATECH e-Handbook of Statistical Methods.

At the beginning of each exercise or case study, I've included a link back to the specific page of the e-Handbook. The e-Handbook can be downloaded in full from the NIST site. The compressed file is over 100Mb (not 43Mb) as stated.

## Software information and conventions

Follow “best practices” of the *tidyverse*

The R session information for this book is shown below:

```
sessionInfo()
```

```
## R version 3.4.3 (2017-11-30)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS High Sierra 10.13.5
##
## Matrix products: default
## BLAS: /Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] stats      graphics  grDevices  utils      datasets  methods   base
##
## other attached packages:
## [1] multcompView_0.1-7 multcomp_1.4-8    TH.data_1.0-8
## [4] MASS_7.3-49        survival_2.42-3   mvtnorm_1.0-7
## [7] lme4_1.1-17         Matrix_1.2-14     broom_0.4.4
## [10] magrittr_1.5        bindrcpp_0.2.2     forcats_0.3.0
## [13] stringr_1.3.0       dplyr_0.7.4        purrr_0.2.4
## [16] readr_1.1.1         tidyr_0.8.0        tibble_1.4.2
## [19] ggplot2_2.2.1       tidyverse_1.2.1
##
## loaded via a namespace (and not attached):
## [1] Rcpp_0.12.16      lubridate_1.7.4    lattice_0.20-35    zoo_1.8-1
## [5] assertthat_0.2.0  rprojroot_1.3-2    digest_0.6.15      psych_1.8.3.3
## [9] utf8_1.1.3        R6_2.2.2           cellranger_1.1.0   plyr_1.8.4
## [13] backports_1.1.2   evaluate_0.10.1    http_1.3.1         pillar_1.2.1
## [17] rlang_0.2.0       lazyeval_0.2.1     readxl_1.0.0       rstudioapi_0.7
## [21] minqa_1.2.4       nloptr_1.0.4       rmarkdown_1.9      labeling_0.3
## [25] splines_3.4.3     foreign_0.8-69     munsell_0.4.3      compiler_3.4.3
## [29] modelr_0.1.1      xfun_0.1           pkgconfig_2.0.1    mnormt_1.5-5
## [33] htmltools_0.3.6   tidyselect_0.2.4   bookdown_0.7       codetools_0.2-15
```

```
## [37] crayon_1.3.4      grid_3.4.3        nlme_3.1-137      jsonlite_1.5
## [41] gtable_0.2.0      scales_0.5.0      cli_1.0.0         stringi_1.1.7
## [45] reshape2_1.4.3    xml2_1.2.0        sandwich_2.4-0    tools_3.4.3
## [49] glue_1.2.0        hms_0.4.2         parallel_3.4.3    yaml_2.1.18
## [53] colorspace_1.3-2  rvest_0.3.2       knitr_1.20        bindr_0.1.1
## [57] haven_1.1.1
```

## Acknowledgements

This book was created using the **bookdown** package (Xie, 2018), which was built on top of R Markdown and **knitr** (Xie, 2015).

Ray James Hoobler  
Salt Lake City, Utah May 2018

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# Chapter 1

## Exploratory Data Analysis

### 1.1 A EDA Example

An EDA/Graphics Example

The Anscombe dataset is an excellent place to start as it will allow us to start using R immediately. The anscombe dataset is part of the **datasets** package and is automatically loaded with RStudio.

```
anscombe
```

```
##      x1 x2 x3 x4      y1      y2      y3      y4
## 1    10 10 10  8    8.04 9.14    7.46    6.58
## 2     8  8  8  8    6.95 8.14    6.77    5.76
## 3    13 13 13  8    7.58 8.74   12.74    7.71
## 4     9  9  9  8    8.81 8.77    7.11    8.84
## 5    11 11 11  8    8.33 9.26    7.81    8.47
## 6    14 14 14  8    9.96 8.10    8.84    7.04
## 7     6  6  6  8    7.24 6.13    6.08    5.25
## 8     4  4  4 19    4.26 3.10    5.39   12.50
## 9    12 12 12  8   10.84 9.13    8.15    5.56
## 10    7  7  7  8    4.82 7.26    6.42    7.91
## 11    5  5  5  8    5.68 4.74    5.73    6.89
```

### 1.2 But first... let's start working in the tidyverse

The tidyverse is described as

an opinionated collection of R packages designed for data science. All packages share an underlying design philosophy, grammar, and data structures.

You can install the **tidyverse** package with

```
install.packages("tidyverse")
```

Once installed, simply load the package:

```
library(tidyverse)
```

Additional details can be found at [tidyverse.org](https://tidyverse.org)

If you have only created charts and graphs using spreadsheets, you will assume the data is ready to plot. It might be nice to have the x1 and y1 values closer together in the table, but we could still select the individual columns and plot the datasets.

We're going to jump right in with the idea of *tidy data*. That each row should be a single observation.

As mentioned in the introduction, this text assumes a basic knowledge of the tidyverse. In this example, we will select the x data from the data frame, rename the column labels, use the `gather()` function to tidy the data. We will then repeat the process for the y data, removing the group names from the data set. The last step is to combine these two data frames into a single data frame we will use for plotting. I'm sure there are more efficient ways to do this; however, the code used to do this manipulation is typical when working with non-tidy data. An added benefit is that the code is readable.

```
x_anscombe <- anscombe %>% # results will be stored into a new object x_anscombe; we start with the o
  dplyr::select(x1, x2, x3, x4) %>% # select the columns we want to work with
  rename(group1 = x1, group2 = x2, group3 = x3, group4 = x4) %>% # rename the values using a generic he
  gather(key = group, value = x_values, group1, group2, group3, group4) # gather the columns into rows
```

```
x_anscombe
```

```
##      group x_values
## 1 group1      10
## 2 group1       8
## 3 group1      13
## 4 group1       9
## 5 group1      11
## 6 group1      14
## 7 group1       6
## 8 group1       4
## 9 group1      12
## 10 group1       7
## 11 group1       5
## 12 group2      10
## 13 group2       8
## 14 group2      13
## 15 group2       9
## 16 group2      11
## 17 group2      14
## 18 group2       6
## 19 group2       4
## 20 group2      12
## 21 group2       7
## 22 group2       5
## 23 group3      10
## 24 group3       8
## 25 group3      13
## 26 group3       9
## 27 group3      11
## 28 group3      14
## 29 group3       6
## 30 group3       4
## 31 group3      12
## 32 group3       7
## 33 group3       5
## 34 group4       8
## 35 group4       8
```

```
## 36 group4      8
## 37 group4      8
## 38 group4      8
## 39 group4      8
## 40 group4      8
## 41 group4     19
## 42 group4      8
## 43 group4      8
## 44 group4      8
```

```
y_anscombe <- anscombe %>%
  dplyr::select(y1, y2, y3, y4) %>%
  gather(key = group, value = y_values, y1, y2, y3, y4) %>% # I don't need to rename the columns as I w
  dplyr::select(y_values)
```

```
y_anscombe
```

```
##      y_values
## 1      8.04
## 2      6.95
## 3      7.58
## 4      8.81
## 5      8.33
## 6      9.96
## 7      7.24
## 8      4.26
## 9     10.84
## 10     4.82
## 11     5.68
## 12     9.14
## 13     8.14
## 14     8.74
## 15     8.77
## 16     9.26
## 17     8.10
## 18     6.13
## 19     3.10
## 20     9.13
## 21     7.26
## 22     4.74
## 23     7.46
## 24     6.77
## 25    12.74
## 26     7.11
## 27     7.81
## 28     8.84
## 29     6.08
## 30     5.39
## 31     8.15
## 32     6.42
## 33     5.73
## 34     6.58
## 35     5.76
## 36     7.71
## 37     8.84
```

```
## 38      8.47
## 39      7.04
## 40      5.25
## 41     12.50
## 42      5.56
## 43      7.91
## 44      6.89
```

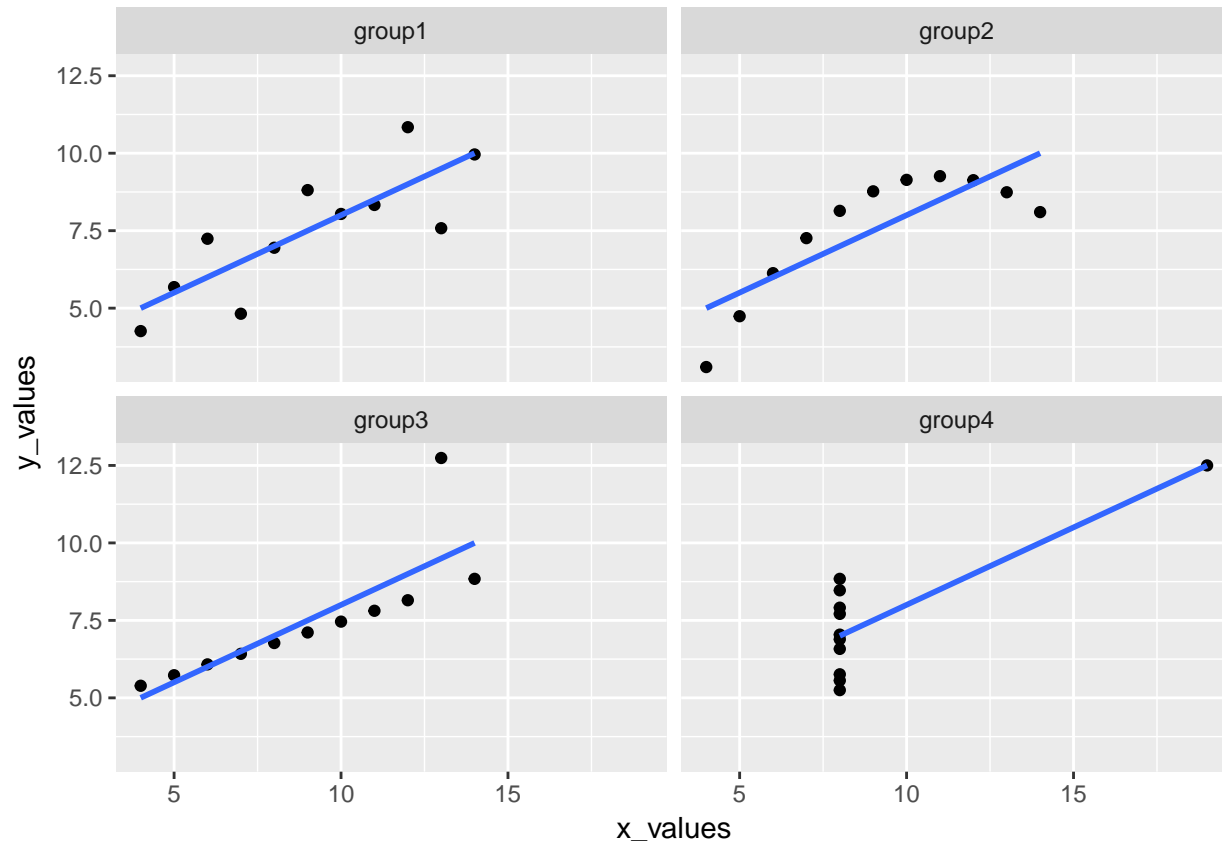
```
anscombe_tidy <- bind_cols(x_anscombe, y_anscombe)
anscombe_tidy
```

```
##      group x_values y_values
## 1  group1      10      8.04
## 2  group1       8      6.95
## 3  group1      13      7.58
## 4  group1       9      8.81
## 5  group1      11      8.33
## 6  group1      14      9.96
## 7  group1       6      7.24
## 8  group1       4      4.26
## 9  group1      12     10.84
## 10 group1       7      4.82
## 11 group1       5      5.68
## 12 group2      10      9.14
## 13 group2       8      8.14
## 14 group2      13      8.74
## 15 group2       9      8.77
## 16 group2      11      9.26
## 17 group2      14      8.10
## 18 group2       6      6.13
## 19 group2       4      3.10
## 20 group2      12      9.13
## 21 group2       7      7.26
## 22 group2       5      4.74
## 23 group3      10      7.46
## 24 group3       8      6.77
## 25 group3      13     12.74
## 26 group3       9      7.11
## 27 group3      11      7.81
## 28 group3      14      8.84
## 29 group3       6      6.08
## 30 group3       4      5.39
## 31 group3      12      8.15
## 32 group3       7      6.42
## 33 group3       5      5.73
## 34 group4       8      6.58
## 35 group4       8      5.76
## 36 group4       8      7.71
## 37 group4       8      8.84
## 38 group4       8      8.47
## 39 group4       8      7.04
## 40 group4       8      5.25
## 41 group4      19     12.50
## 42 group4       8      5.56
## 43 group4       8      7.91
```

```
## 44 group4      8      6.89
```

While this may seem like a lot of work to make a new table—which is much harder to read—this method allows us to exploit the **grammar of graphics** used by the **ggplot2** package.

```
ggplot(anscombe_tidy, aes(x_values, y_values)) +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE) +
  facet_wrap(~group)
```



It may not be immediately obvious from the plots, but the slope and intercept for each line are identical. We can calculate these values for each dataset using the linear model function, `lm()`.

```
lm(y1 ~ x1, data = anscombe)
```

```
##
## Call:
## lm(formula = y1 ~ x1, data = anscombe)
##
## Coefficients:
## (Intercept)      x1
##      3.0001      0.5001
```

```
lm(y2 ~ x2, data = anscombe)
```

```
##
## Call:
## lm(formula = y2 ~ x2, data = anscombe)
##
## Coefficients:
```

```
## (Intercept)          x2
##      3.001          0.500
lm(y3 ~ x3, data = anscombe)

##
## Call:
## lm(formula = y3 ~ x3, data = anscombe)
##
## Coefficients:
## (Intercept)          x3
##      3.0025          0.4997
lm(y4 ~ x4, data = anscombe)

##
## Call:
## lm(formula = y4 ~ x4, data = anscombe)
##
## Coefficients:
## (Intercept)          x4
##      3.0017          0.4999
```

The calculated slope and intercept are the same (at least to three significant figures); the use of EDA allows us to differentiate the data quickly.

## 1.3 Common graphical analysis used in the e-Handbook

Four techniques are routinely used in the e-Handbook for preliminary EDA. These four charts are routinely displayed as a “4-plot.” Each technique will be presented in the following sub-sections.

- Run sequence plot
- Lag plot
- Histogram
- Normal probability plot

## 1.4 Case studies from chapter 1 of the NIST/SEMATECH e-Handbook

### 1.4.1 Normal random numbers

Normal Random Numbers

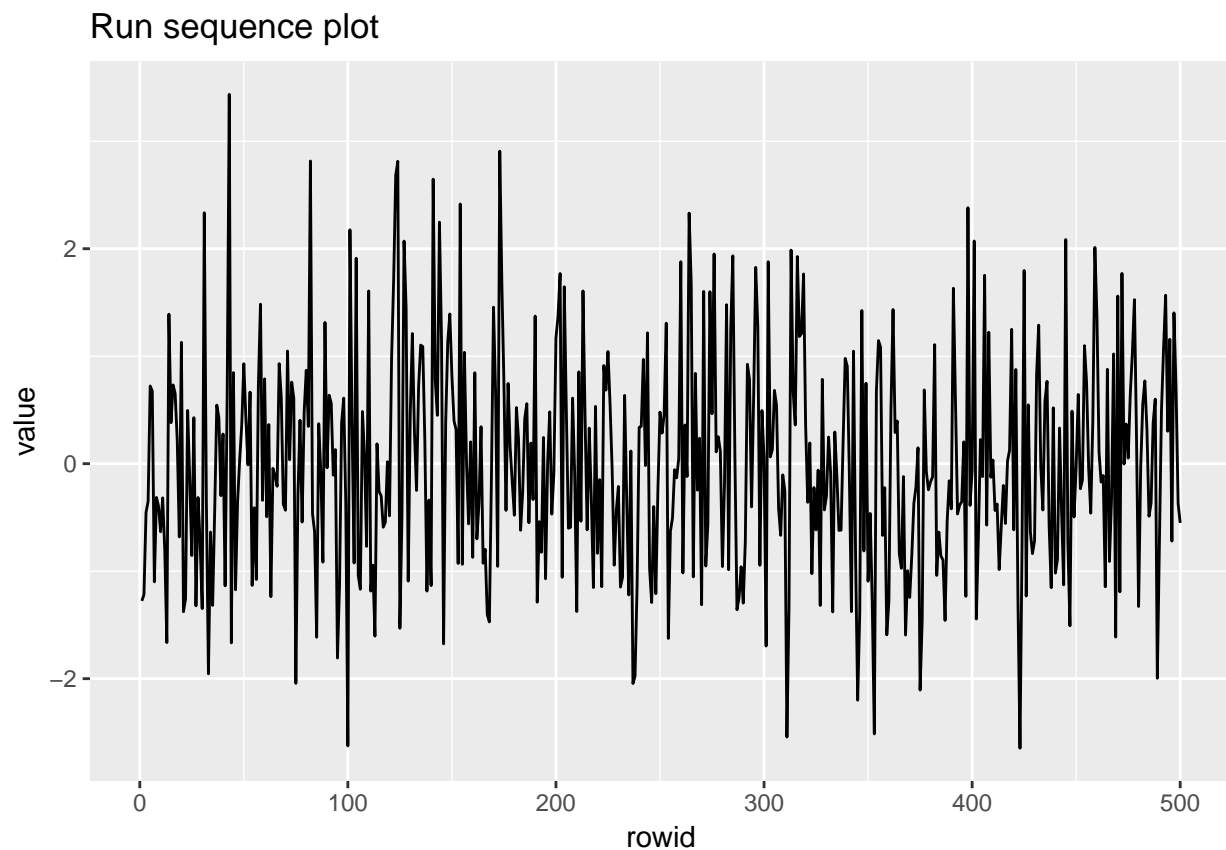
```
normal_random_numbers <- scan("NIST data/RANDN.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()

normal_random_numbers

## # A tibble: 500 x 2
##   rowid value
##   <int> <dbl>
## 1      1 -1.28
```

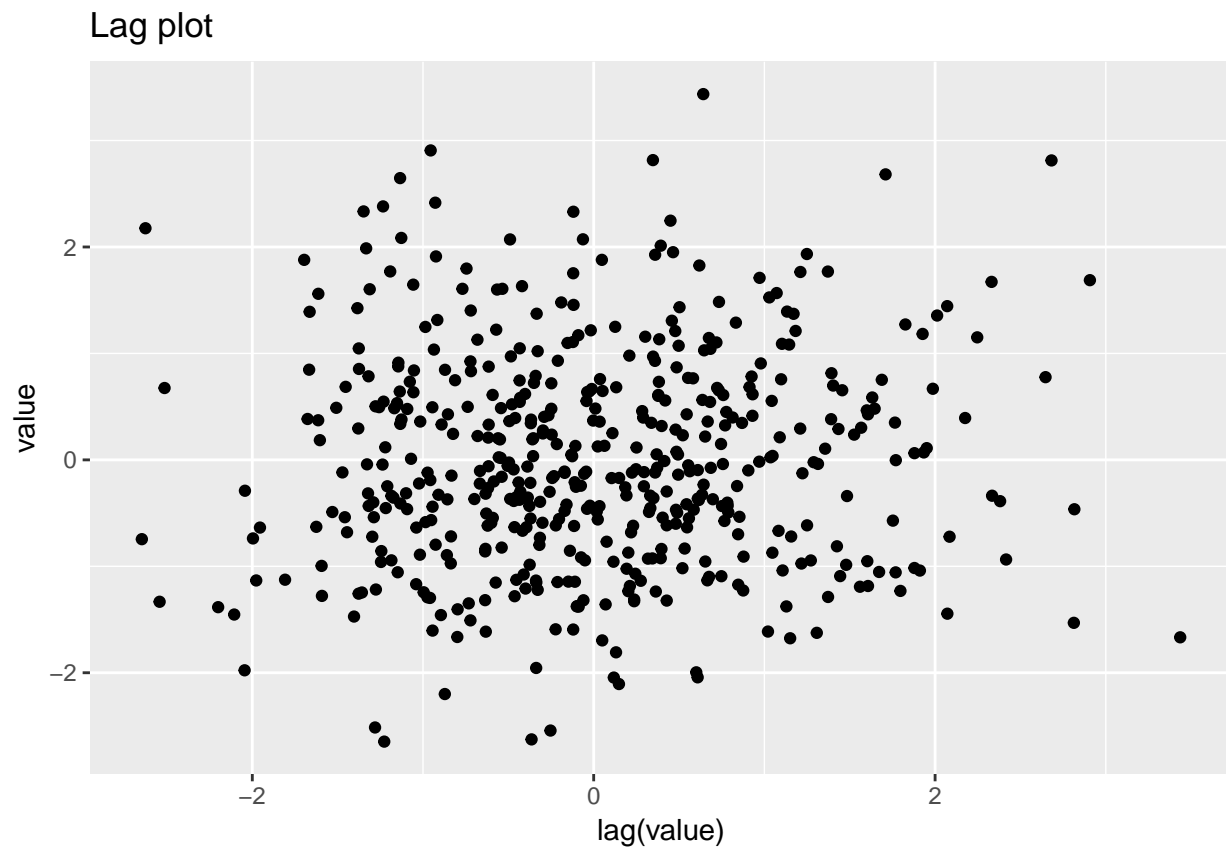
```
## 2      2 -1.22
## 3      3 -0.453
## 4      4 -0.350
## 5      5  0.723
## 6      6  0.676
## 7      7 -1.10
## 8      8 -0.314
## 9      9 -0.394
## 10     10 -0.633
## # ... with 490 more rows
```

```
ggplot(normal_random_numbers, aes(rowid, value)) +
  geom_line() +
  labs(title = "Run sequence plot")
```



```
ggplot(normal_random_numbers, aes(lag(value), value)) +
  geom_point() +
  labs(title = "Lag plot")
```

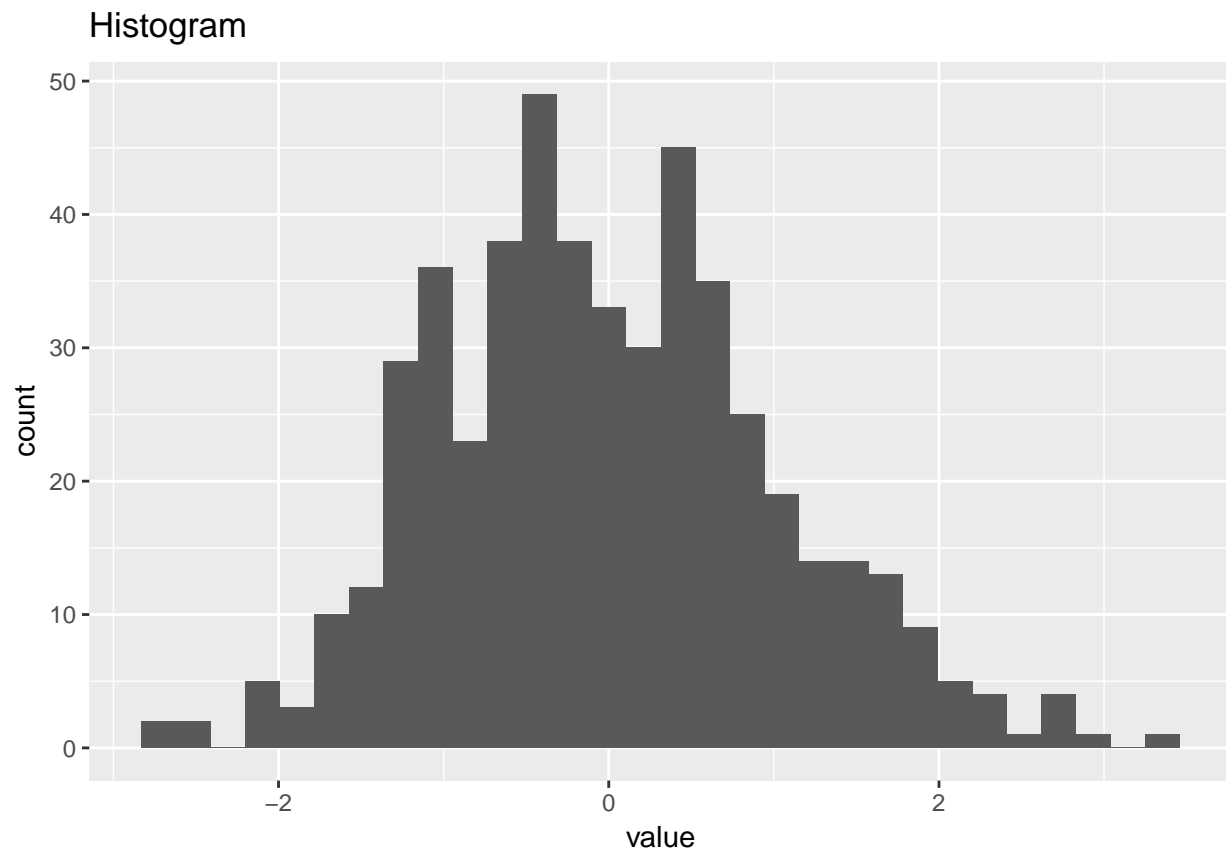
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



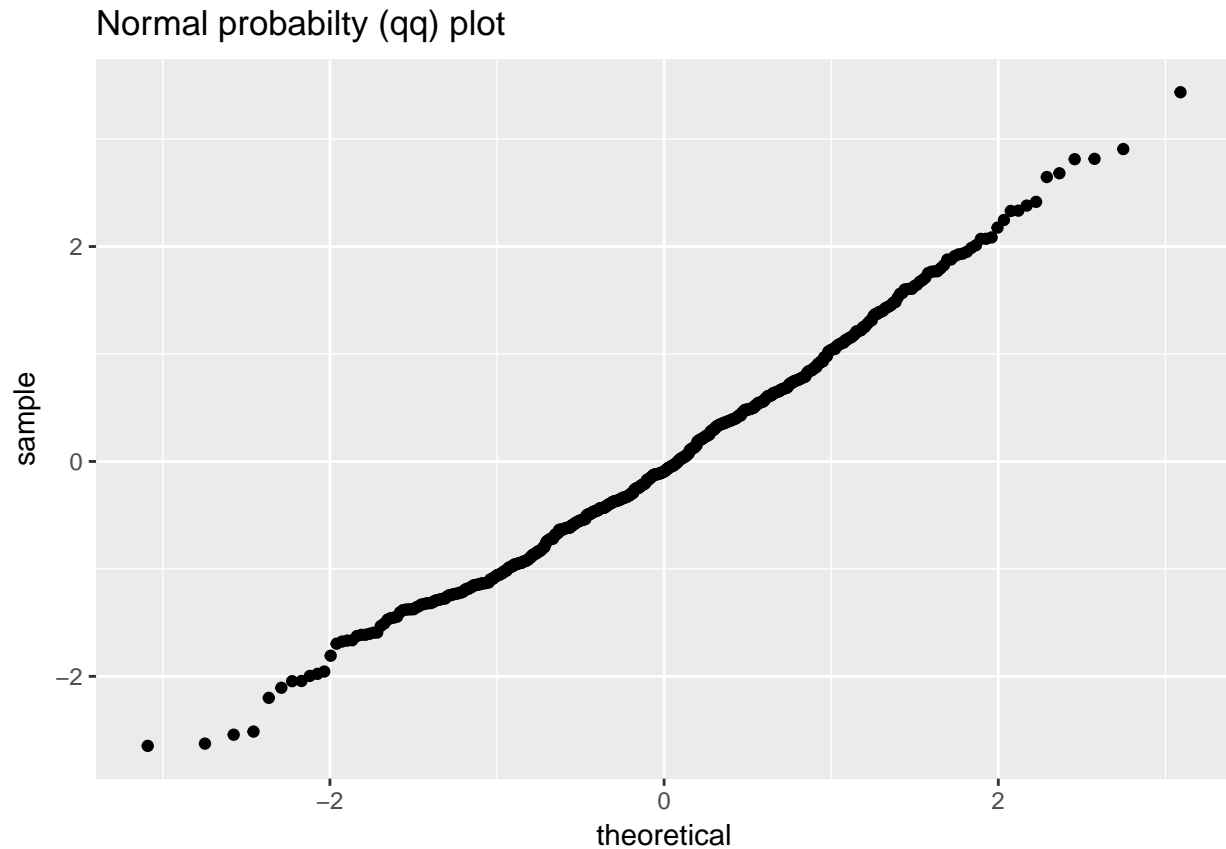
```
ggplot(normal_random_numbers, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```





```
ggplot(normal_random_numbers, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.2 Uniform random numbers

Uniform Random Numbers

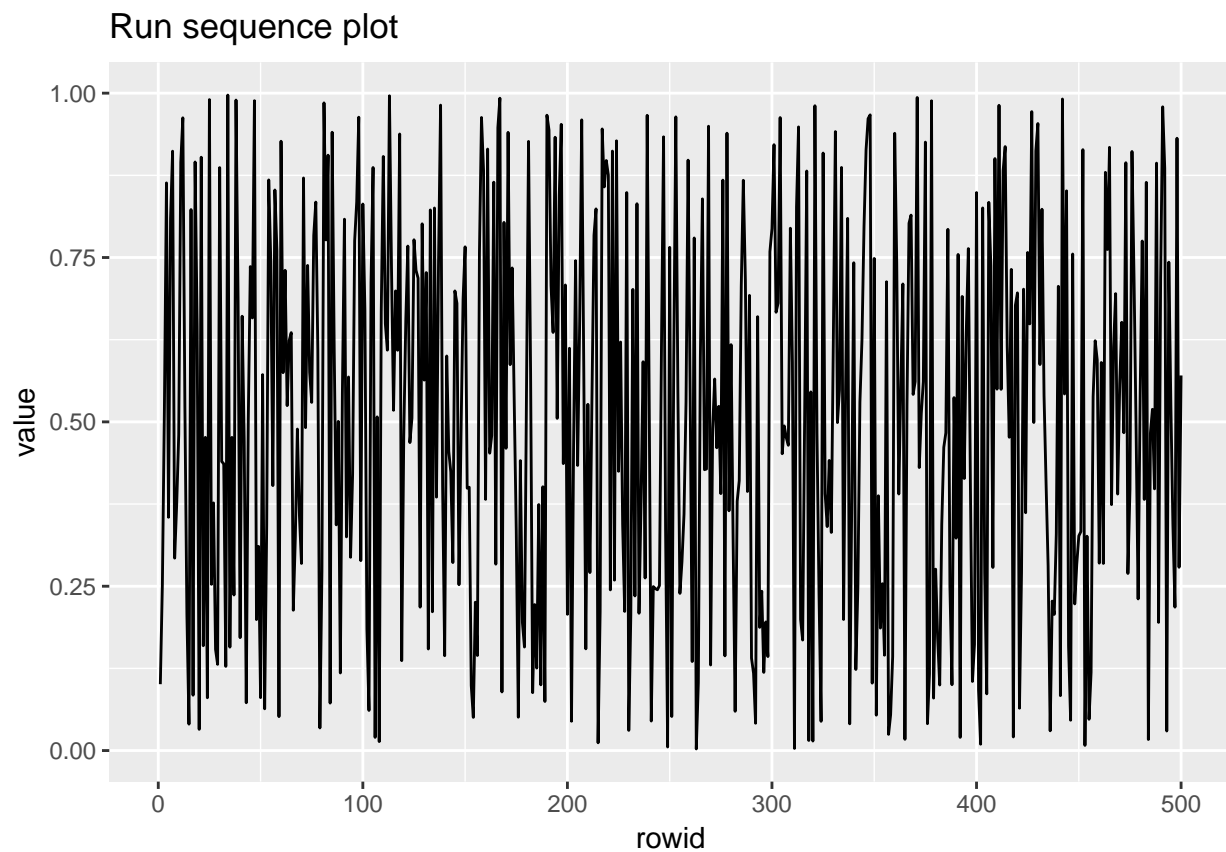
```
uniform_random_numbers <- scan("NIST data/RANDU.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()

uniform_random_numbers
```

```
## # A tibble: 500 x 2
##   rowid value
##   <int> <dbl>
## 1     1 0.101
## 2     2 0.253
## 3     3 0.520
## 4     4 0.863
## 5     5 0.355
## 6     6 0.810
## 7     7 0.912
## 8     8 0.293
## 9     9 0.375
## 10    10 0.481
## # ... with 490 more rows
```

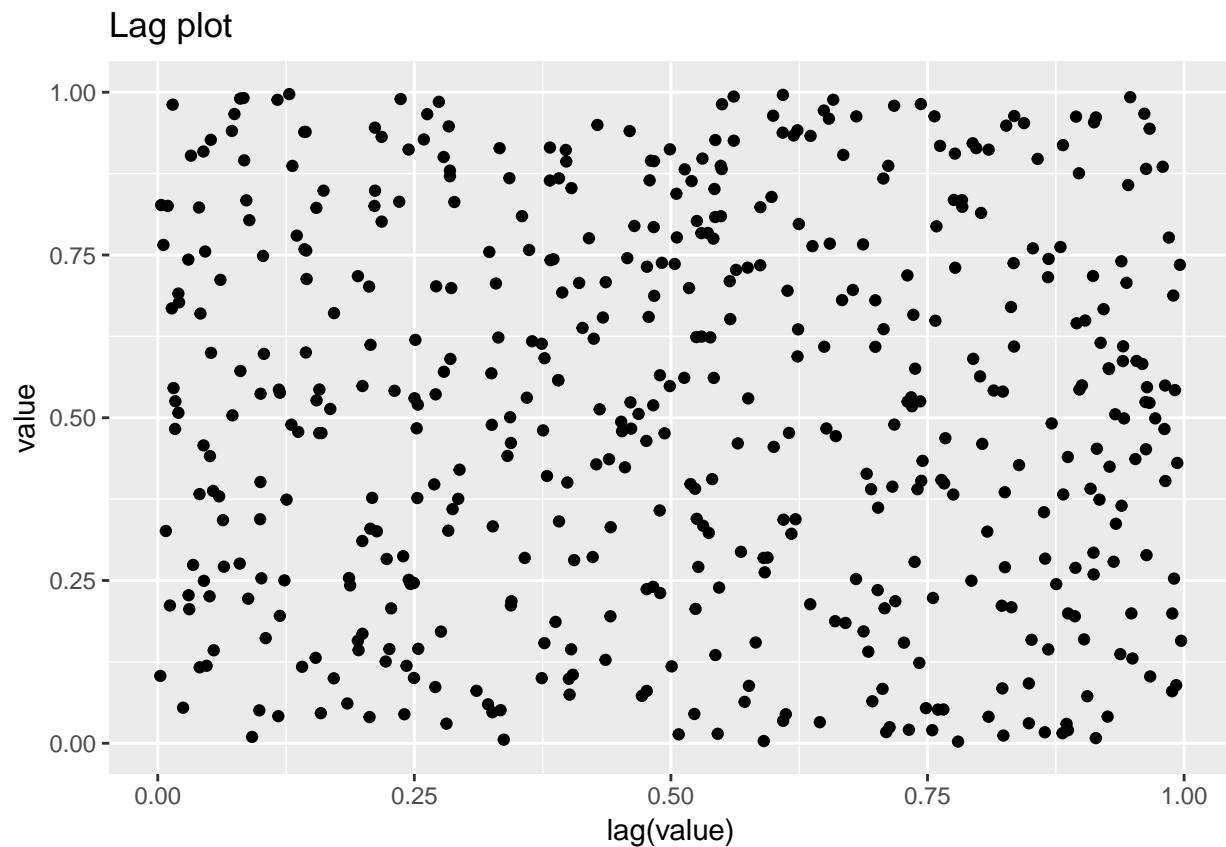
```
ggplot(uniform_random_numbers, aes(rowid, value)) +
  geom_line() +
```

```
labs(title = "Run sequence plot")
```



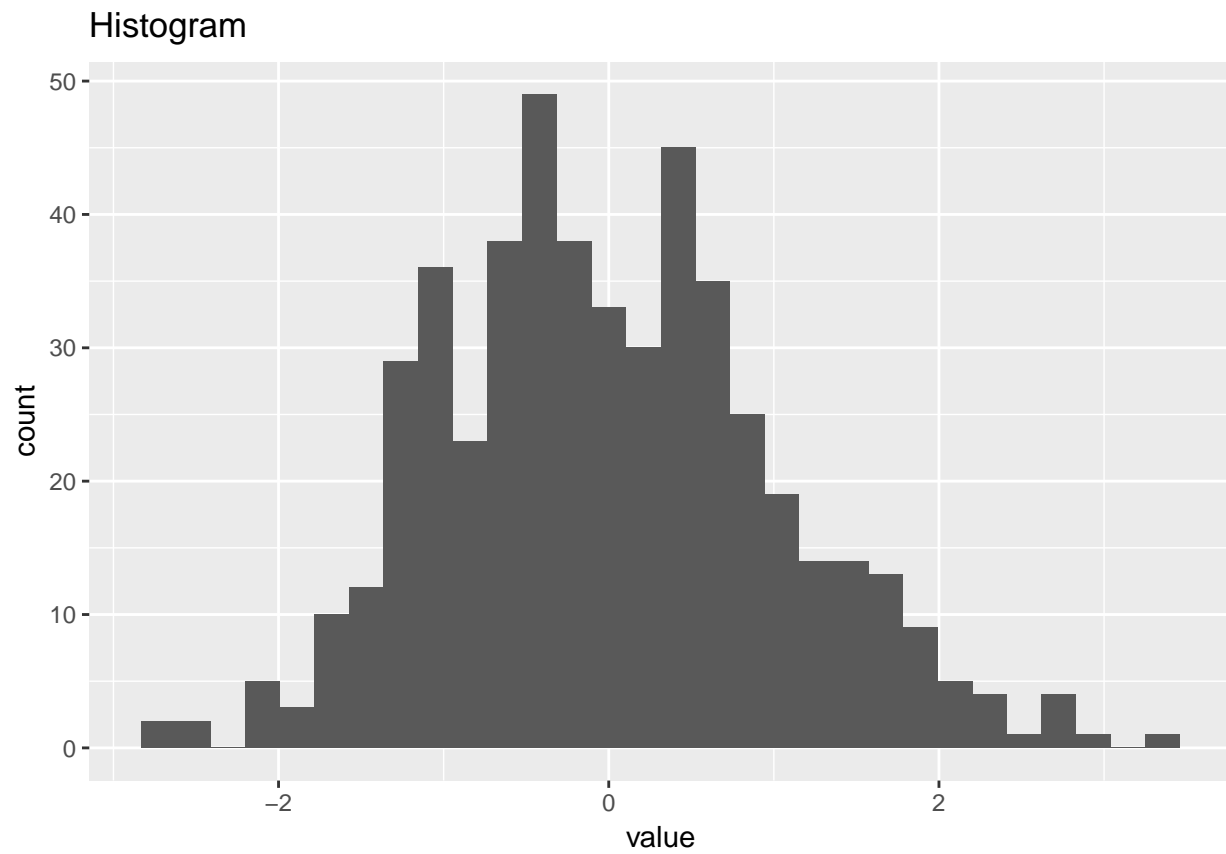
```
ggplot(uniform_random_numbers, aes(lag(value), value)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

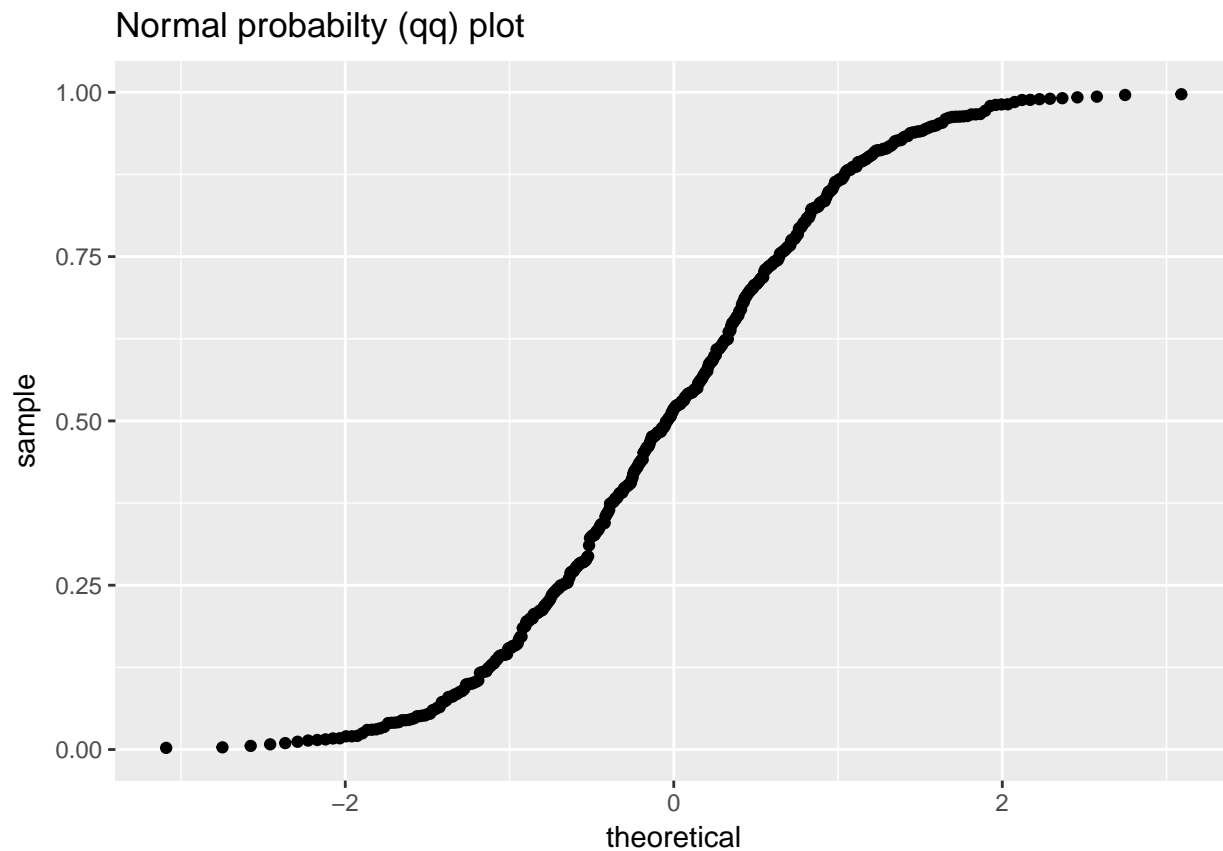


```
ggplot(normal_random_numbers, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(uniform_random_numbers, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.3 Random walk

Random Walk

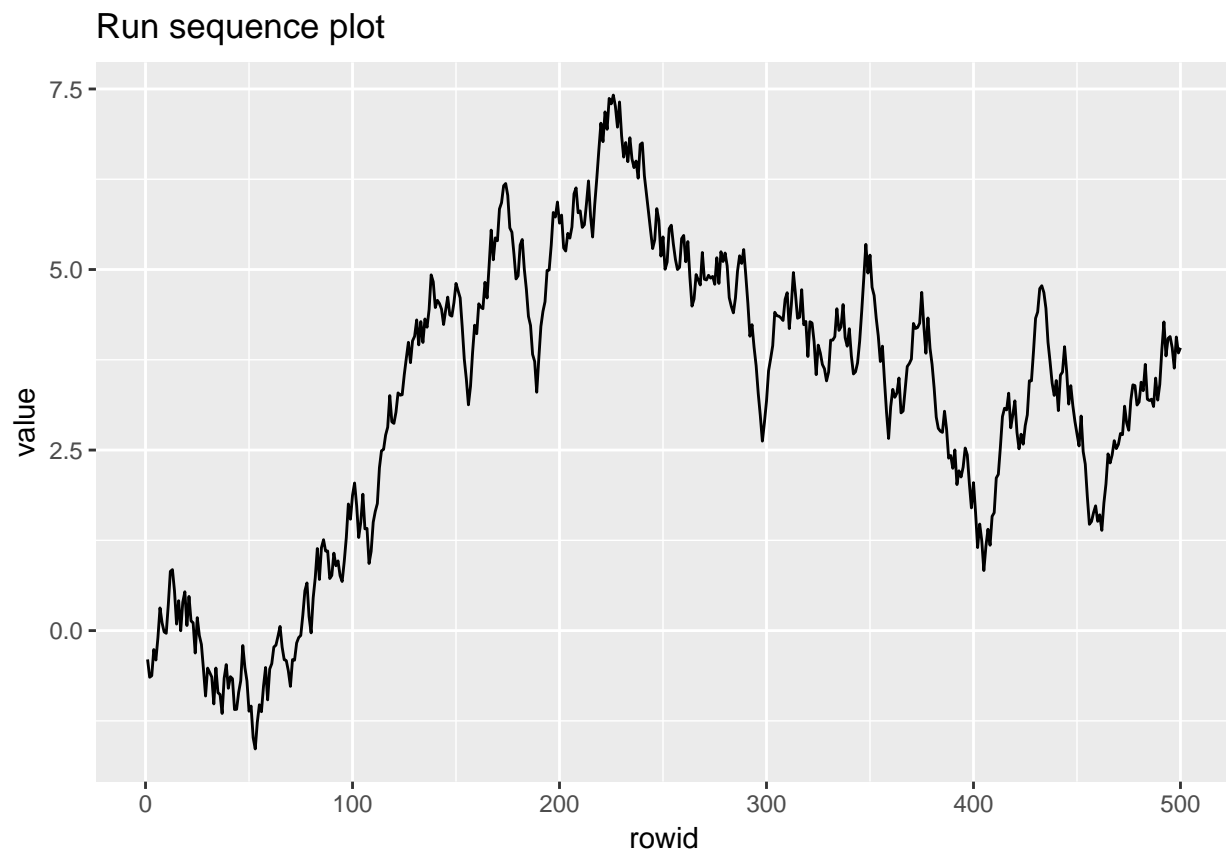
```
random_walk <- scan("NIST data/RANDWALK.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()
```

random\_walk

```
## # A tibble: 500 x 2
##   rowid  value
##   <int> <dbl>
## 1     1 -0.399
## 2     2 -0.646
## 3     3 -0.626
## 4     4 -0.262
## 5     5 -0.407
## 6     6 -0.0976
## 7     7  0.314
## 8     8  0.107
## 9     9 -0.0177
## 10    10 -0.0371
## # ... with 490 more rows
```

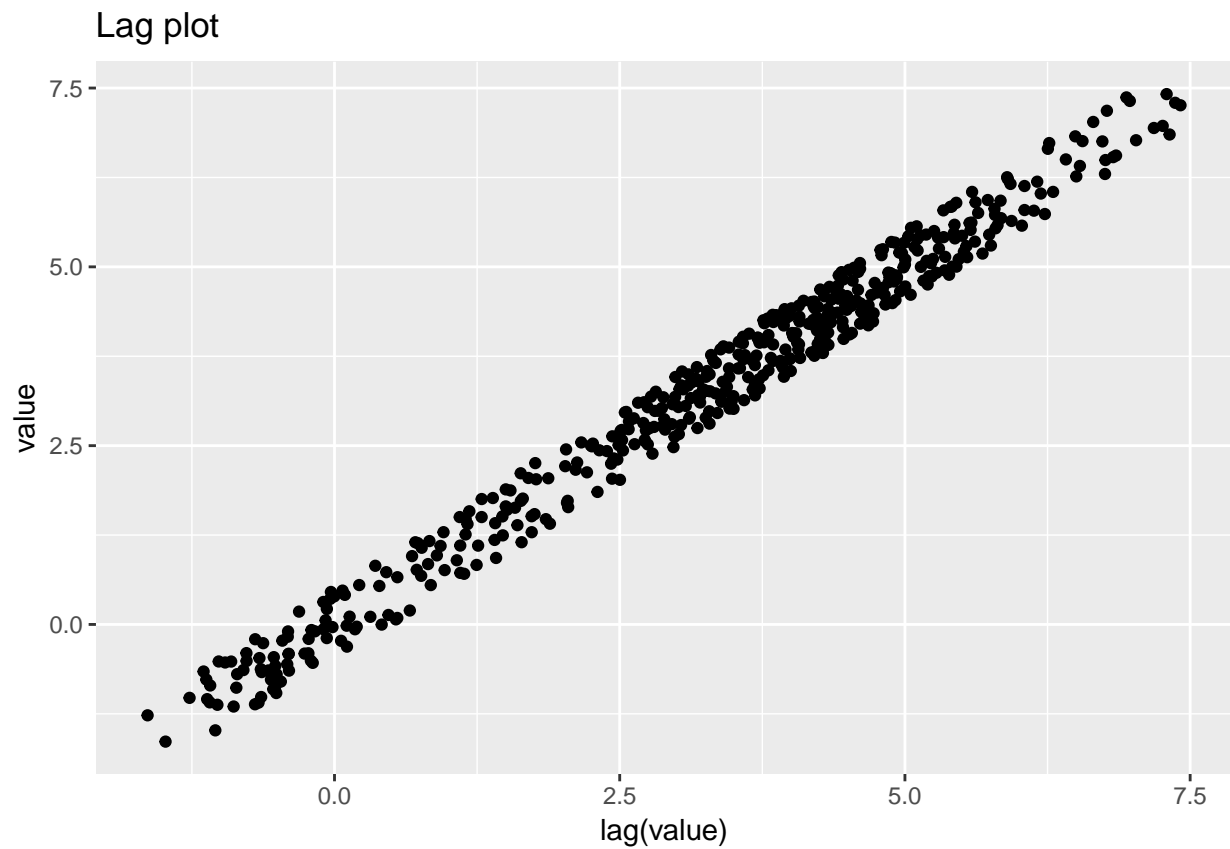
```
ggplot(random_walk, aes(rowid, value)) +
  geom_line() +
```

```
labs(title = "Run sequence plot")
```



```
ggplot(random_walk, aes(lag(value), value)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

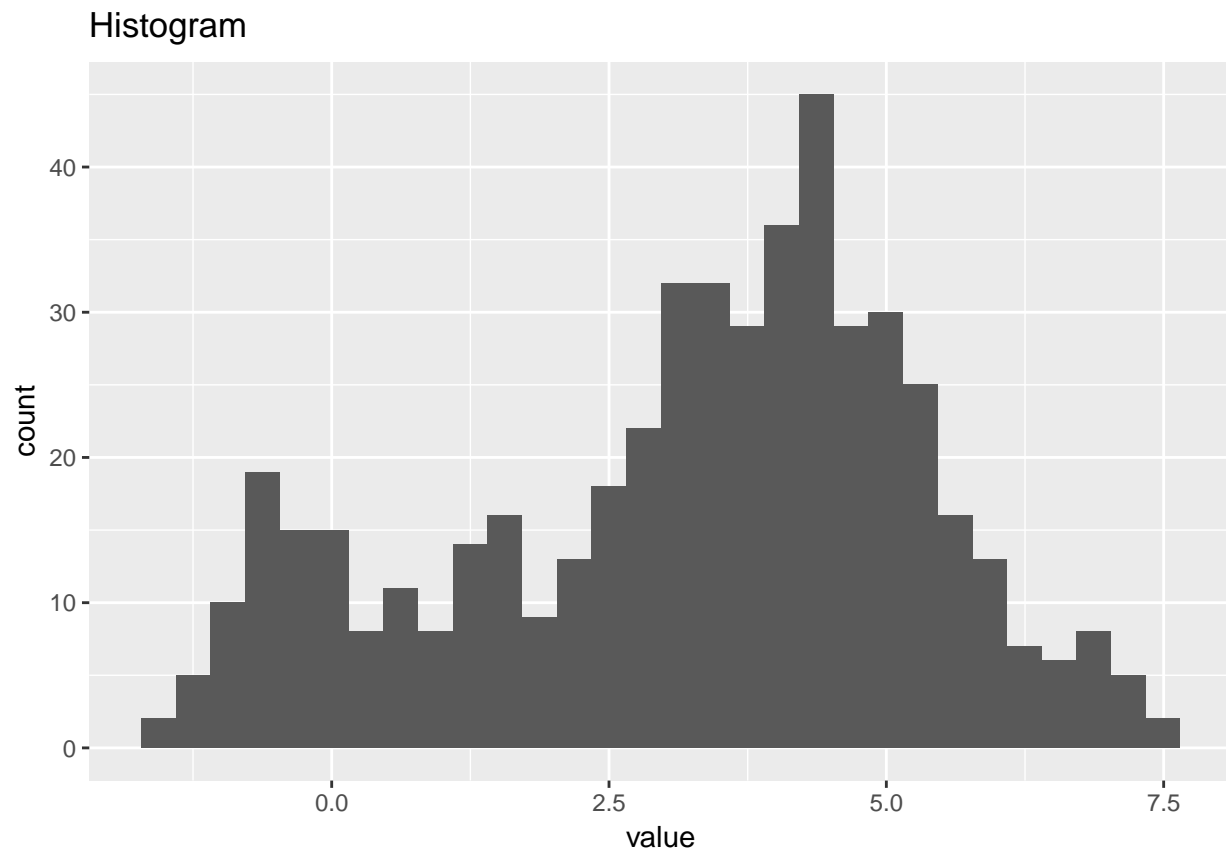
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



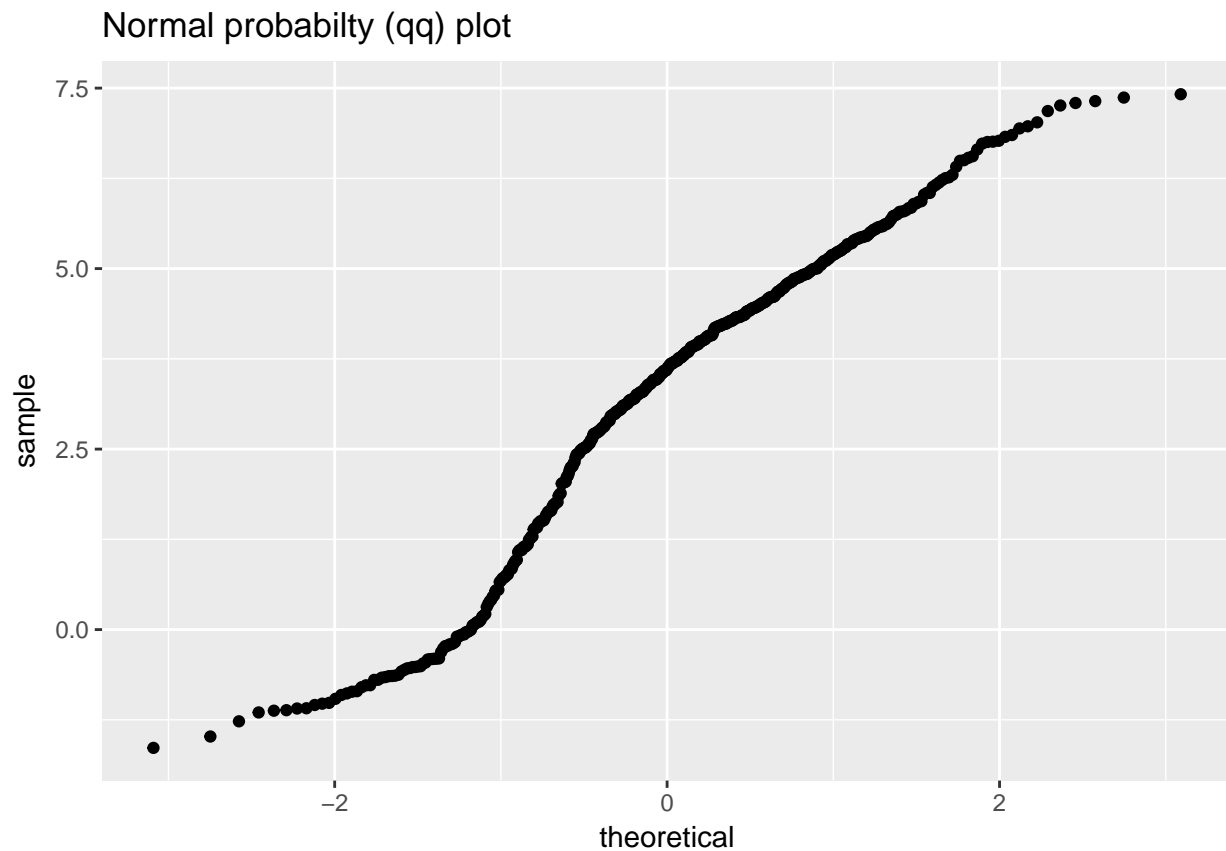
```
ggplot(random_walk, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```





```
ggplot(random_walk, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



#### 1.4.4 Beam deflections

Beam Deflections

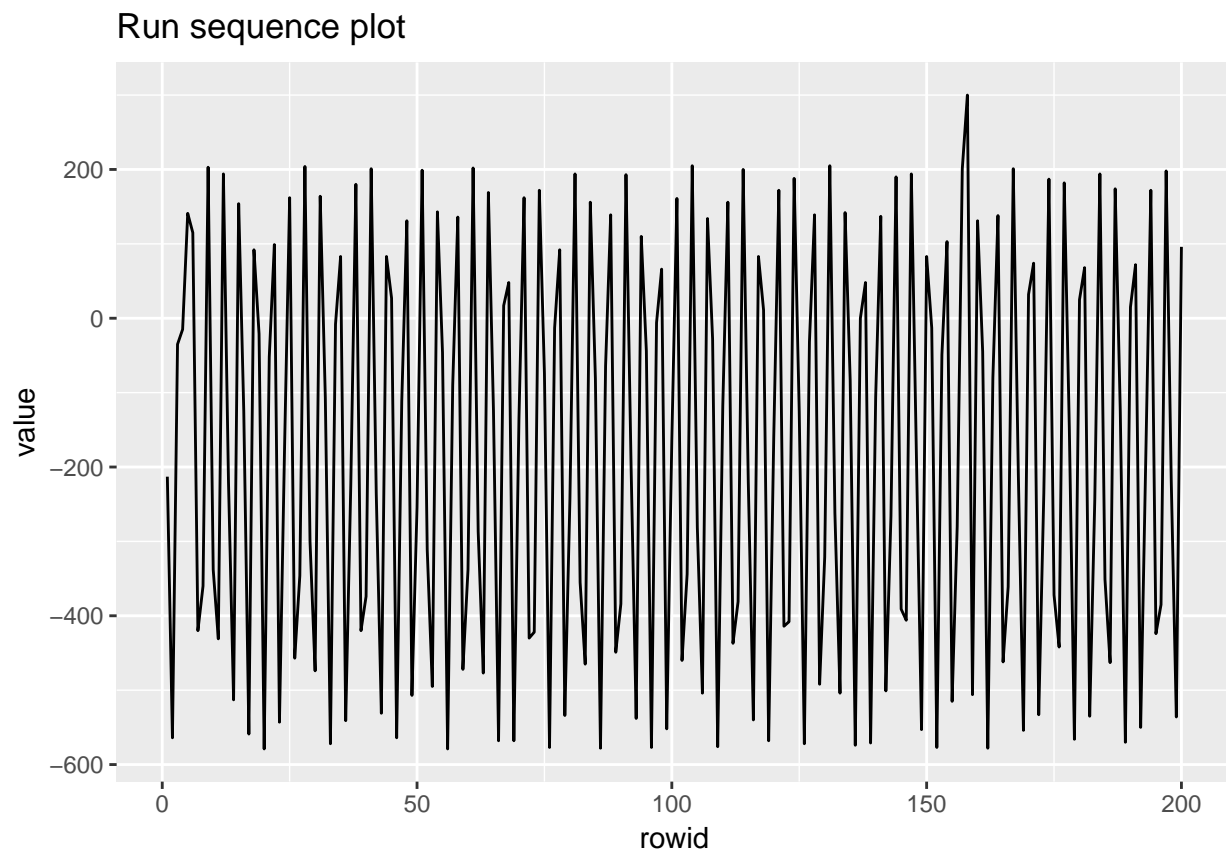
```
beam_deflections <- scan("NIST data/LEW.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()
```

```
beam_deflections
```

```
## # A tibble: 200 x 2
##   rowid value
##   <int> <dbl>
## 1     1 -213.
## 2     2 -564.
## 3     3  -35.
## 4     4  -15.
## 5     5  141.
## 6     6  115.
## 7     7 -420.
## 8     8 -360.
## 9     9  203.
## 10    10 -338.
## # ... with 190 more rows
```

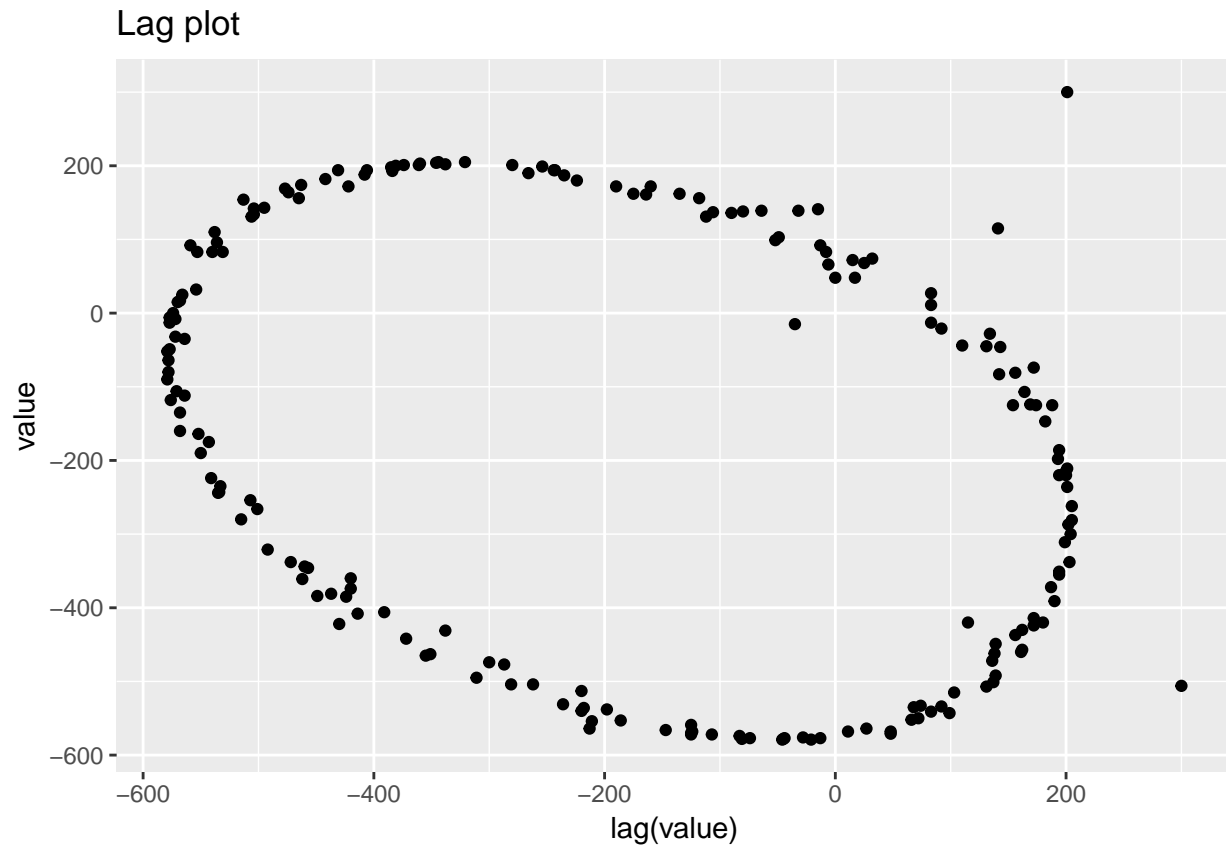
```
ggplot(beam_deflections, aes(rowid, value)) +
  geom_line() +
```

```
labs(title = "Run sequence plot")
```



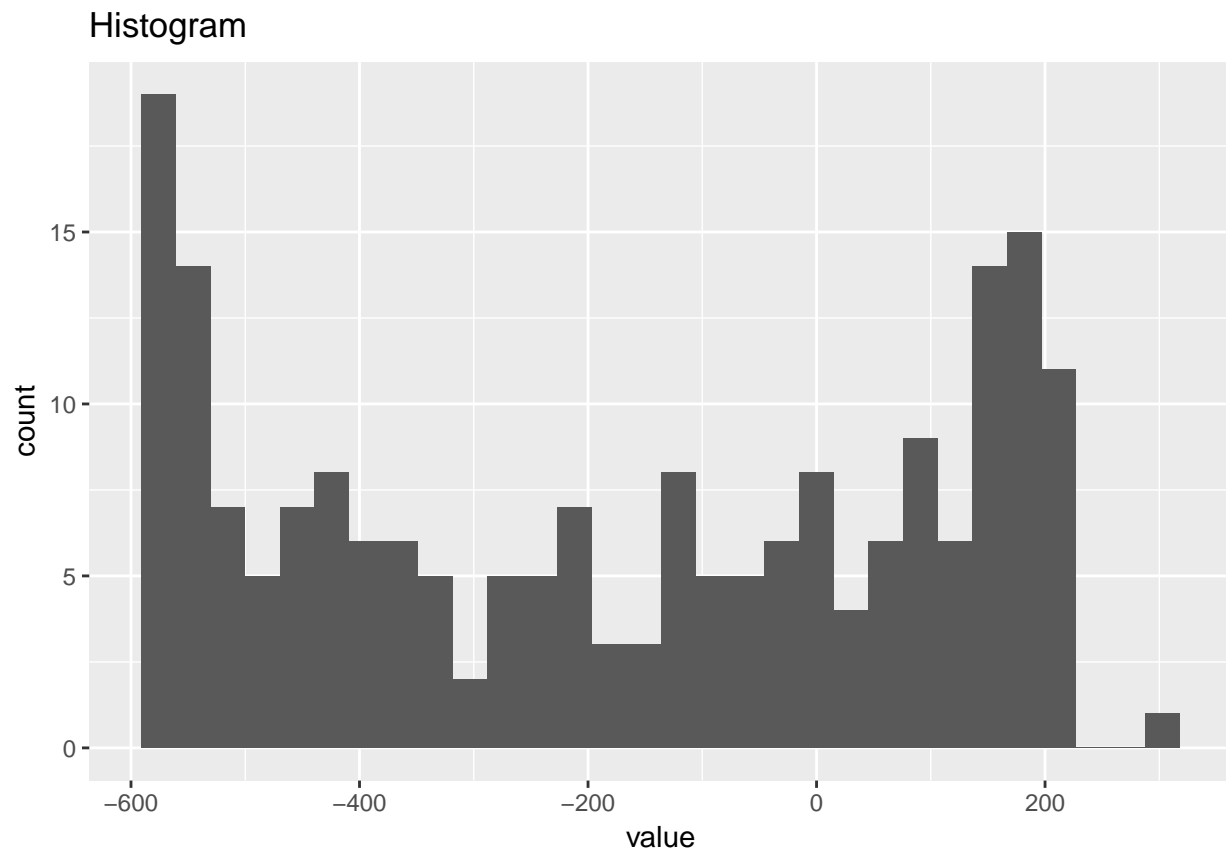
```
ggplot(beam_deflections, aes(lag(value), value)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

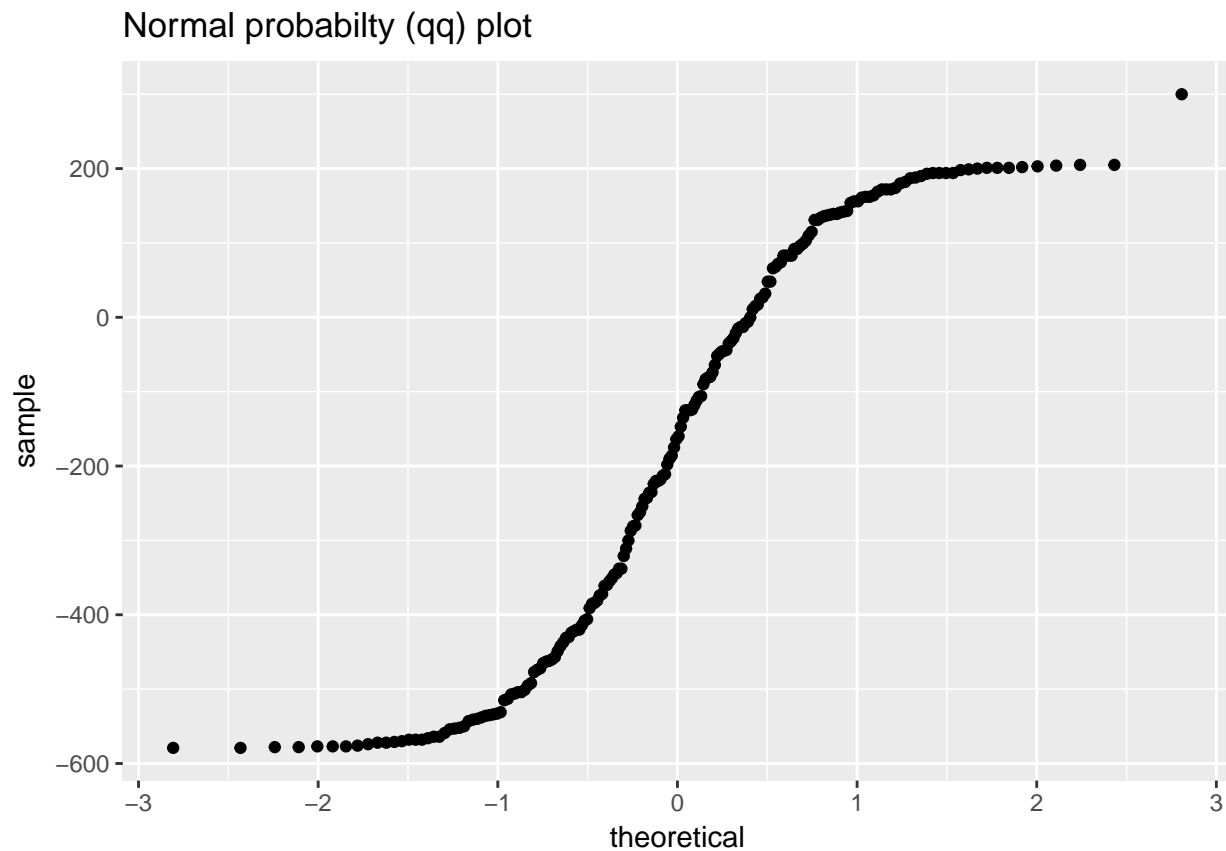


```
ggplot(bean_deflections, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(bean_deflections, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.5 Filter transmittance

Filter Transmittance

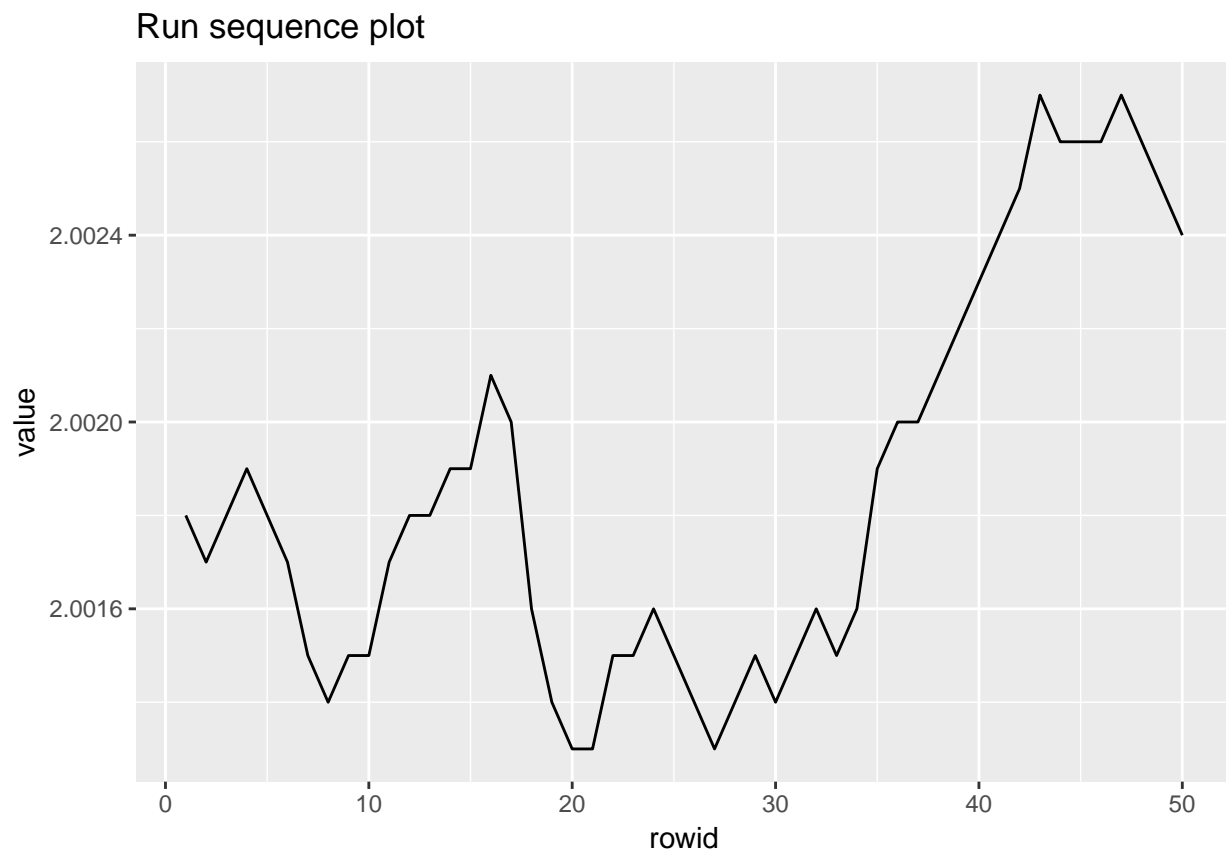
```
filter_transmittance <- scan("NIST data/MAVRO.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()
```

```
filter_transmittance
```

```
## # A tibble: 50 x 2
##   rowid value
##   <int> <dbl>
## 1     1  2.00
## 2     2  2.00
## 3     3  2.00
## 4     4  2.00
## 5     5  2.00
## 6     6  2.00
## 7     7  2.00
## 8     8  2.00
## 9     9  2.00
## 10    10  2.00
## # ... with 40 more rows
```

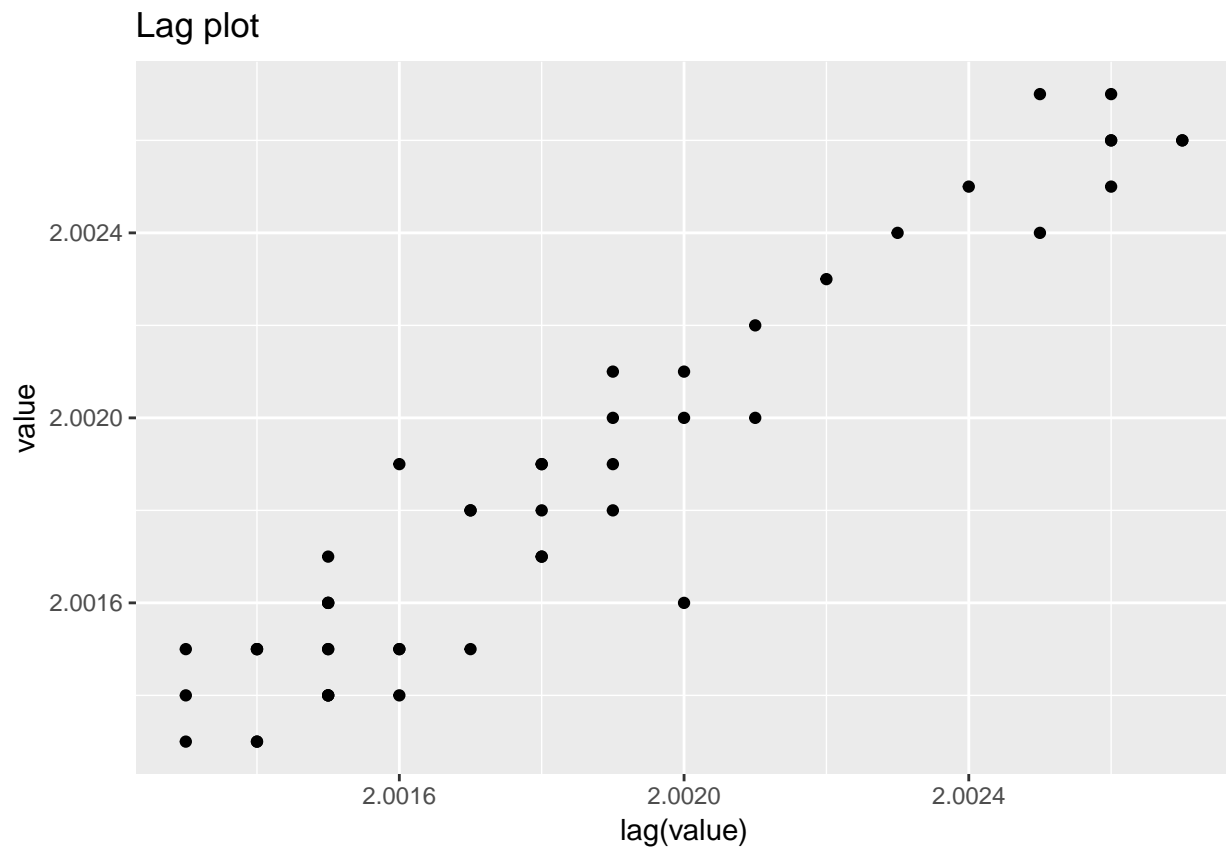
```
ggplot(filter_transmittance, aes(rowid, value)) +
  geom_line() +
```

```
labs(title = "Run sequence plot")
```



```
ggplot(filter_transmittance, aes(lag(value), value)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

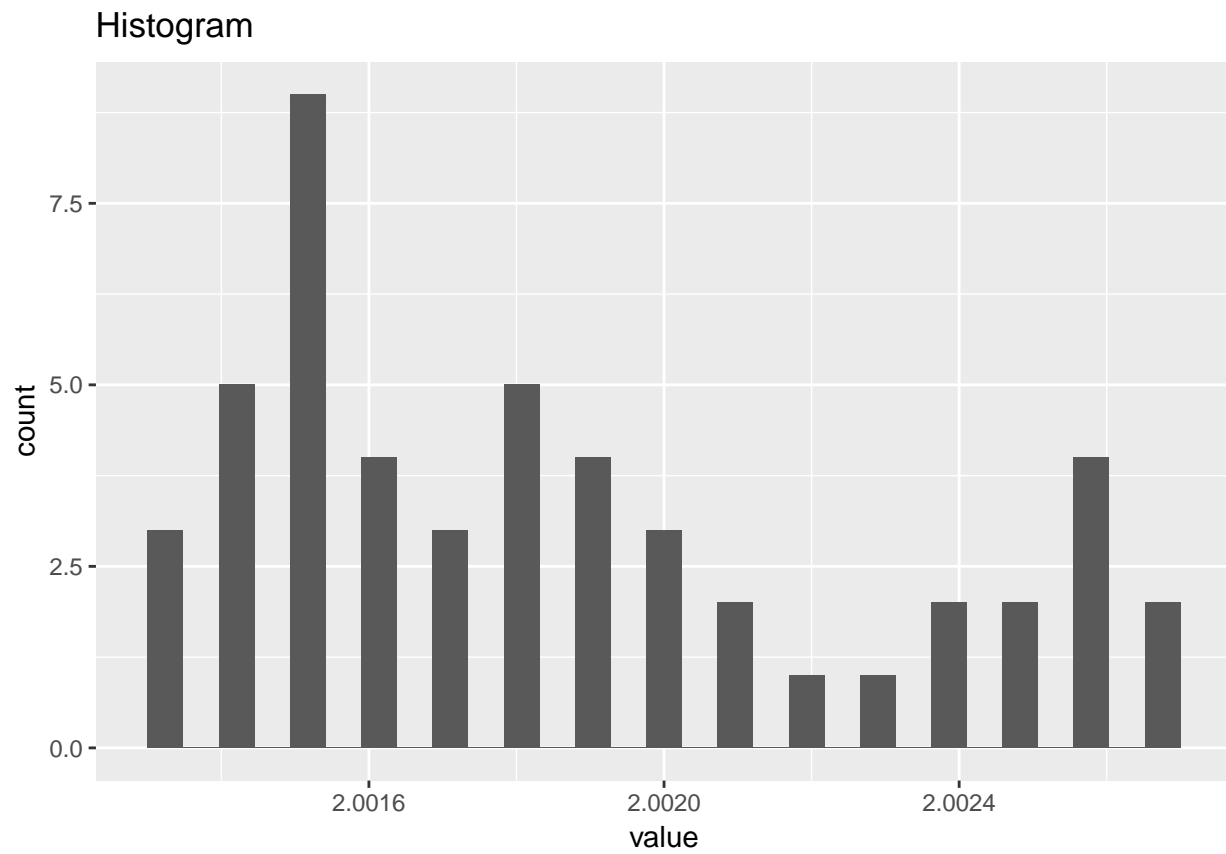
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



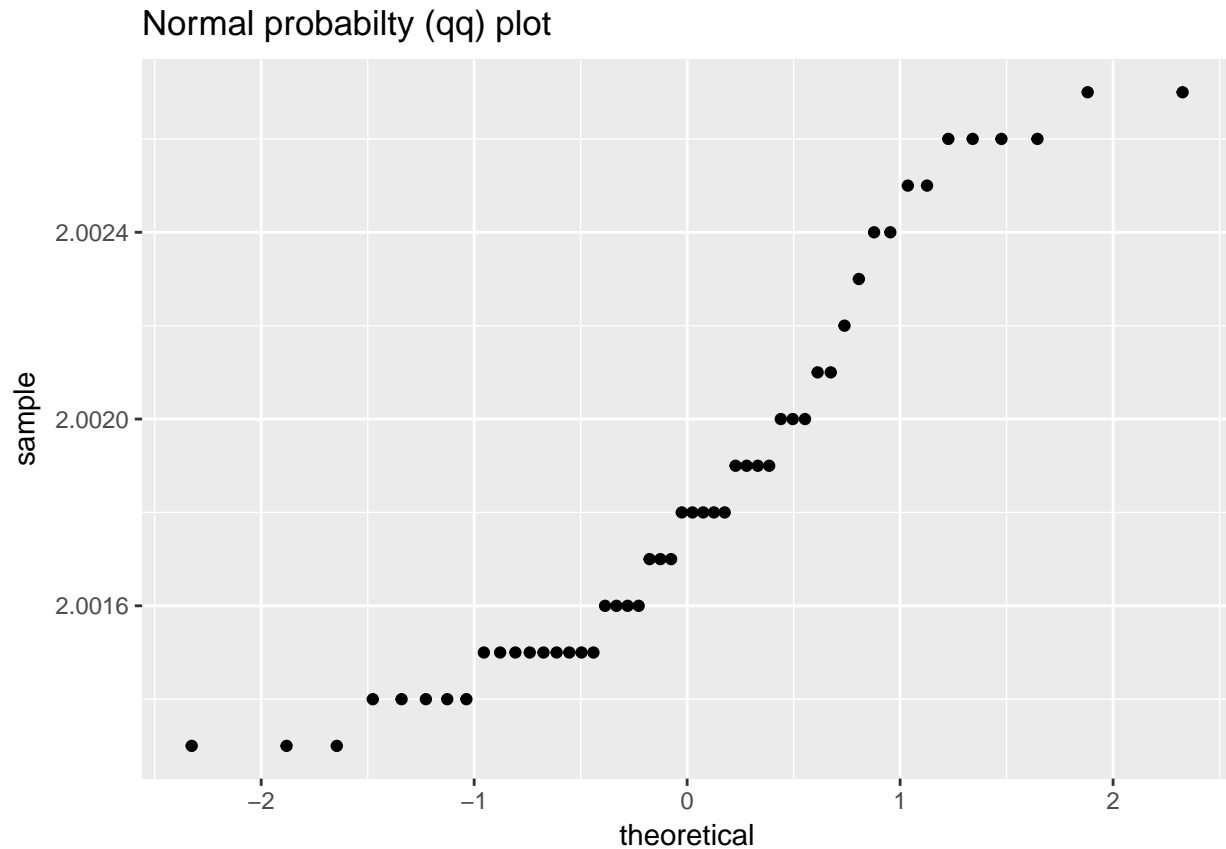
```
ggplot(filter_transmittance, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```





```
ggplot(filter_transmittance, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.6 Standard resistor

Standard Resistor

```
standard_resistor <- read_table2("NIST data/DZIUBA1.DAT", skip = 25, col_names = FALSE) %>%
  rowid_to_column() %>%
  rename(month = X1, day = X2, year = X3, resistance = X4)
```

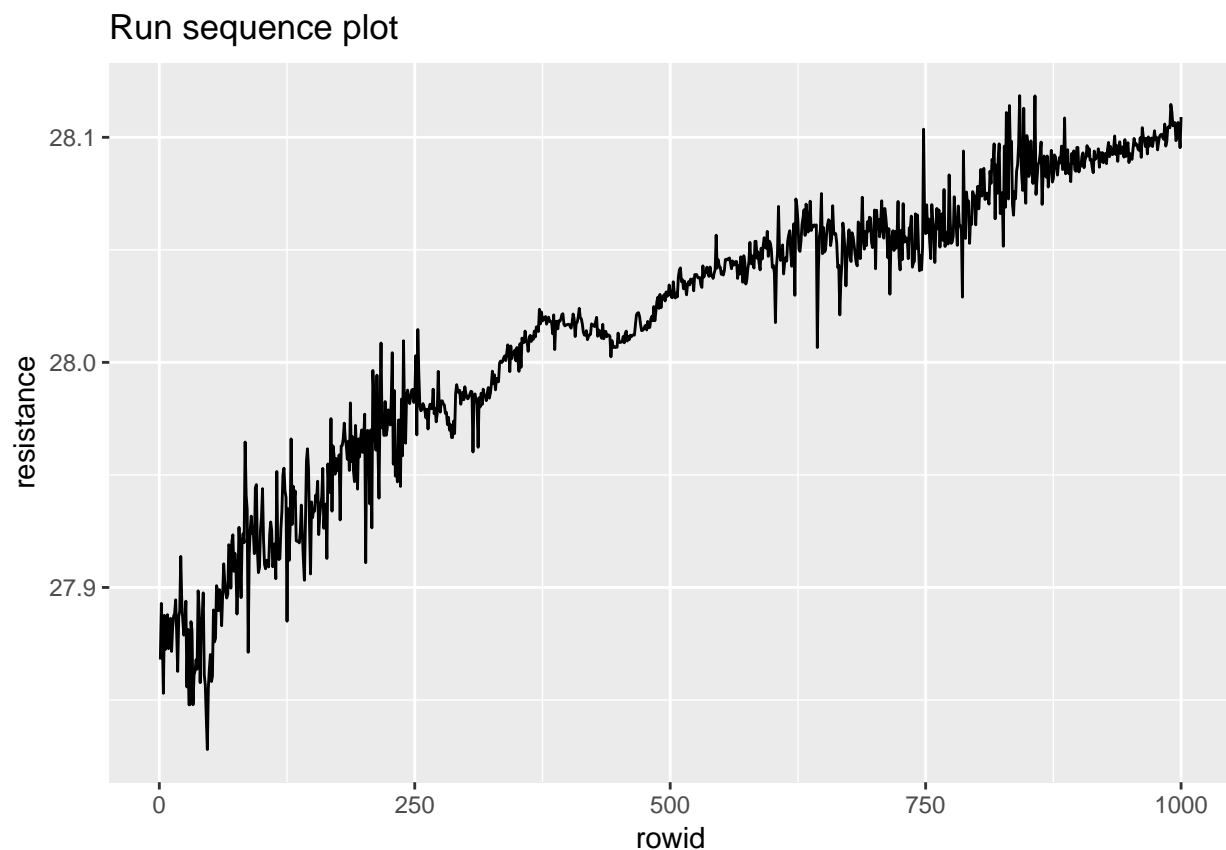
```
## Parsed with column specification:
## cols(
##   X1 = col_character(),
##   X2 = col_character(),
##   X3 = col_integer(),
##   X4 = col_double()
## )
```

```
standard_resistor
```

```
## # A tibble: 1,000 x 5
##   rowid month day   year resistance
##   <int> <chr> <chr> <int>     <dbl>
## 1     1  1 2     5      80      27.9
## 2     2  2 2    12      80      27.9
## 3     3  3 2    13      80      27.9
## 4     4  4 2    14      80      27.9
## 5     5  5 2    28      80      27.9
## 6     6  6 2    28      80      27.9
```

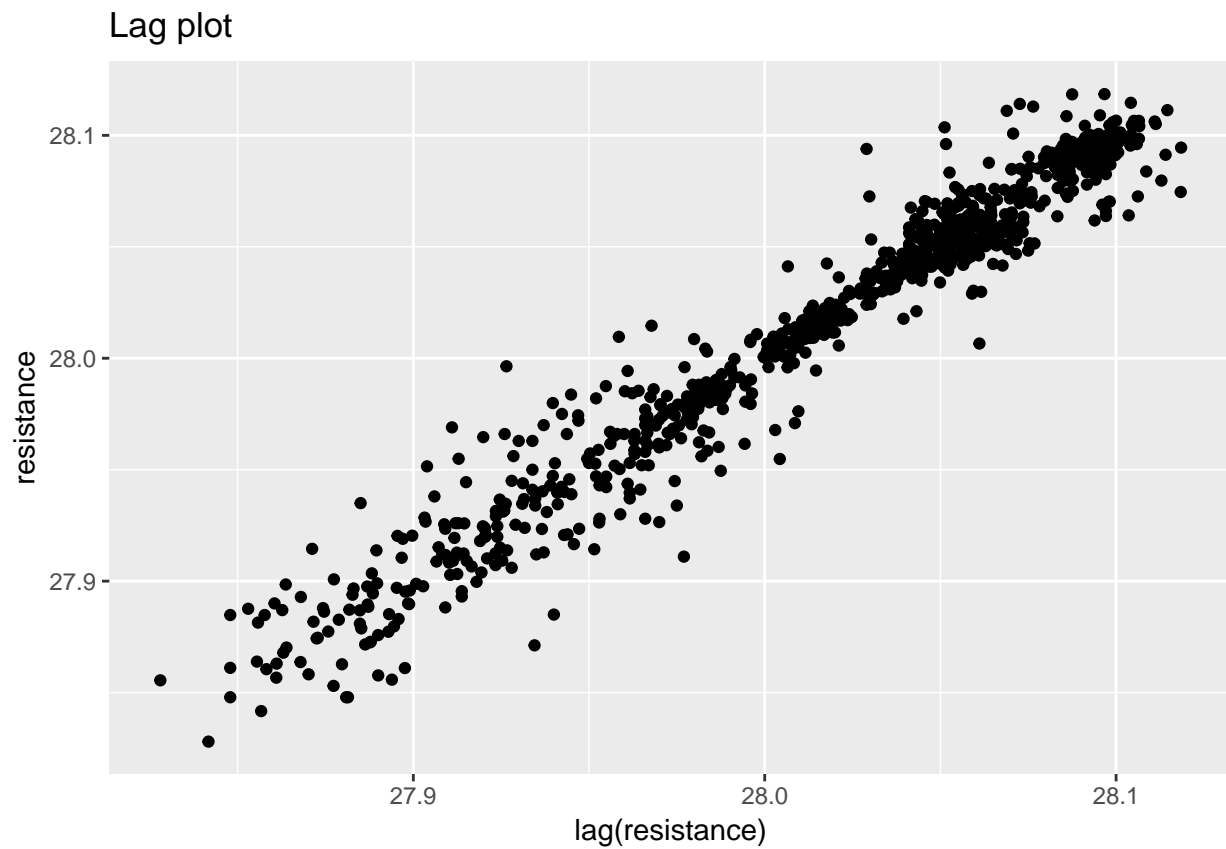
```
## 7      7 3      21      80      27.9
## 8      8 3      24      80      27.9
## 9      9 4       3      80      27.9
## 10     10 4       3      80      27.9
## # ... with 990 more rows
```

```
ggplot(standard_resistor, aes(rowid, resistance)) +
  geom_line() +
  labs(title = "Run sequence plot")
```



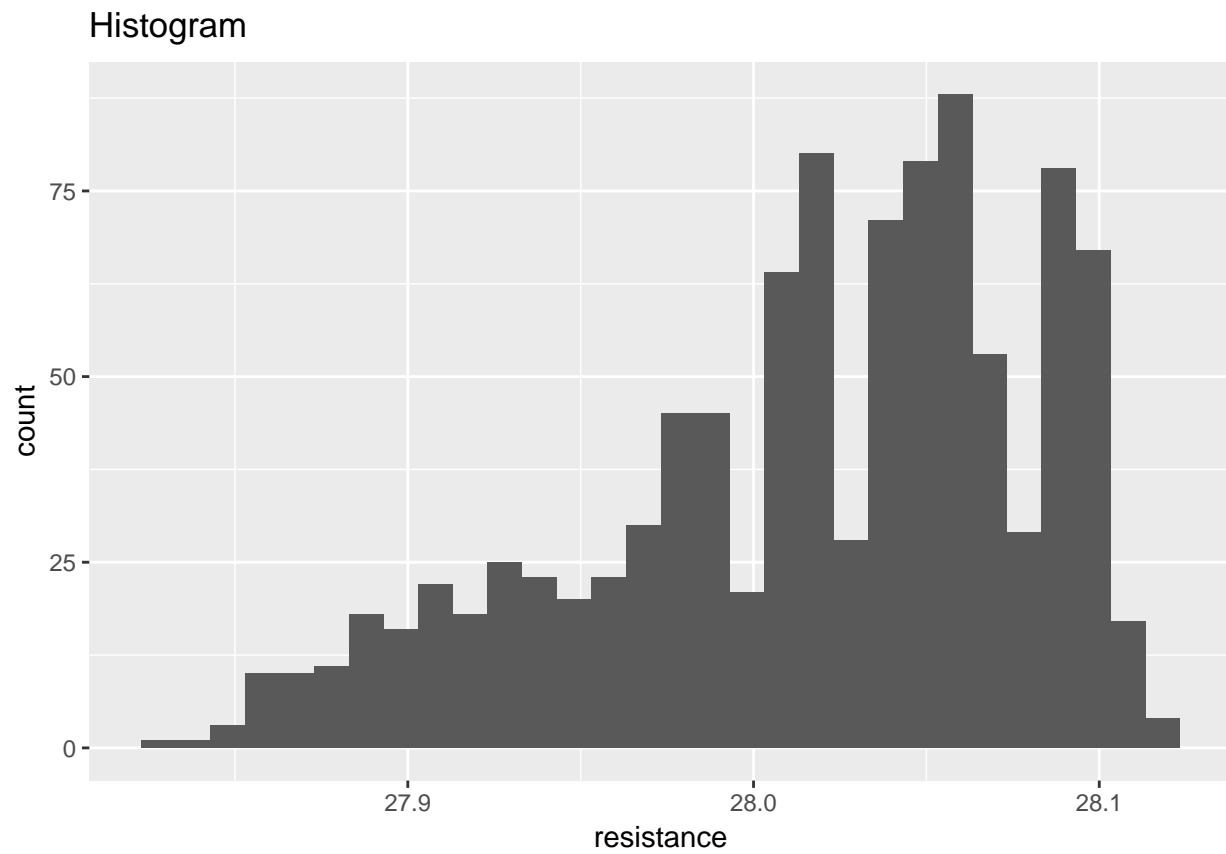
```
ggplot(standard_resistor, aes(lag(resistance), resistance)) +
  geom_point() +
  labs(title = "Lag plot")
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

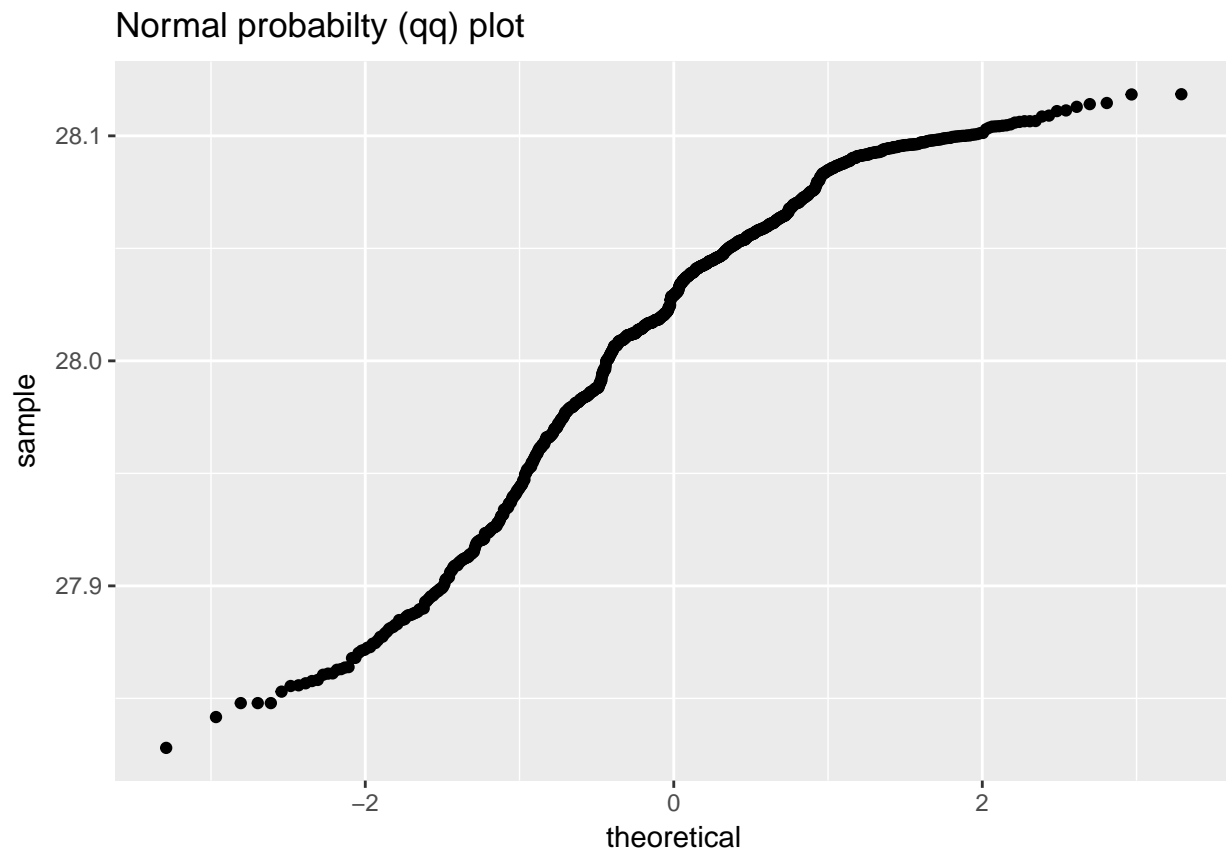


```
ggplot(standard_resistor, aes(resistance)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(standard_resistor, aes(sample = resistance)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.7 Heat flow meter 1

Heat Flow Meter 1

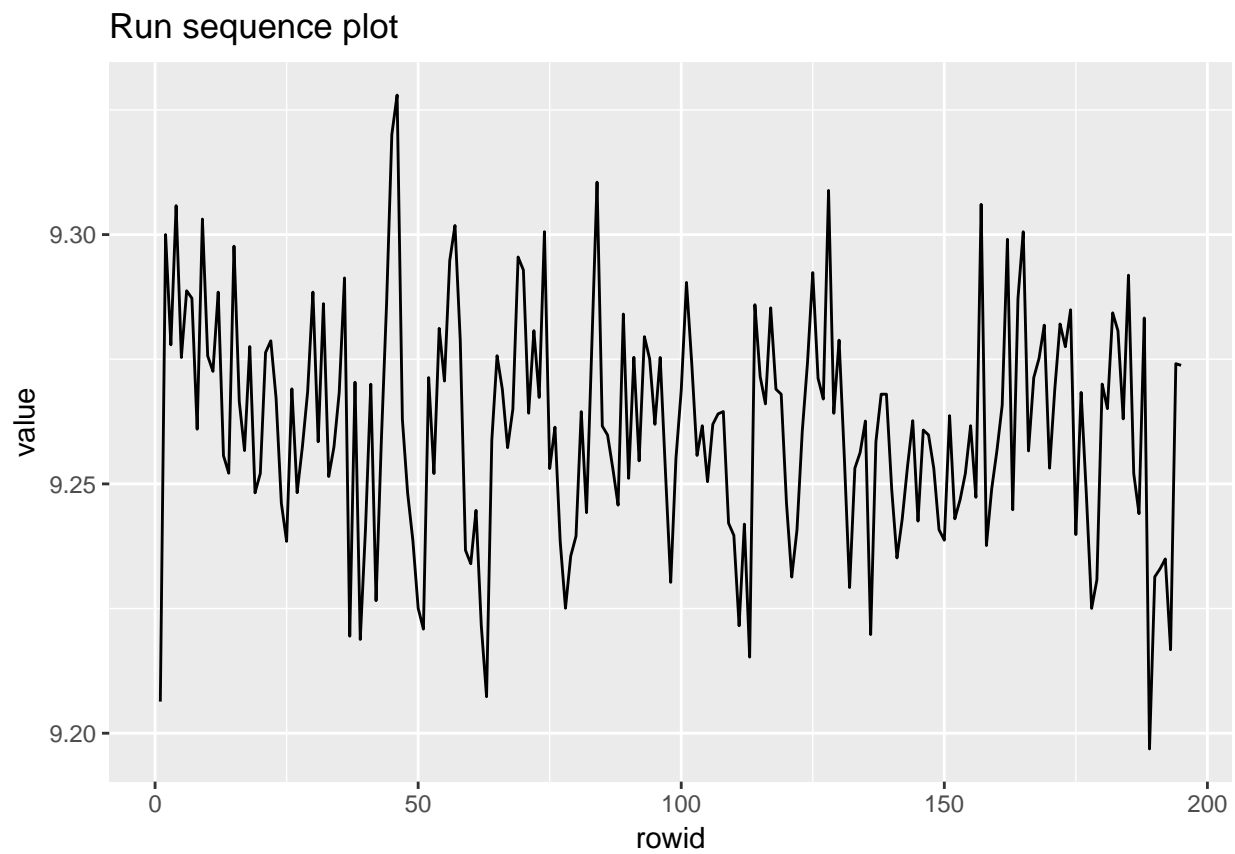
```
heat_flow_meter1 <- scan("NIST data/ZARR13.DAT", skip = 25) %>%
  as.tibble() %>%
  rowid_to_column()
```

```
heat_flow_meter1
```

```
## # A tibble: 195 x 2
##   rowid value
##   <int> <dbl>
## 1     1  9.21
## 2     2  9.30
## 3     3  9.28
## 4     4  9.31
## 5     5  9.28
## 6     6  9.29
## 7     7  9.29
## 8     8  9.26
## 9     9  9.30
## 10    10  9.28
## # ... with 185 more rows
```

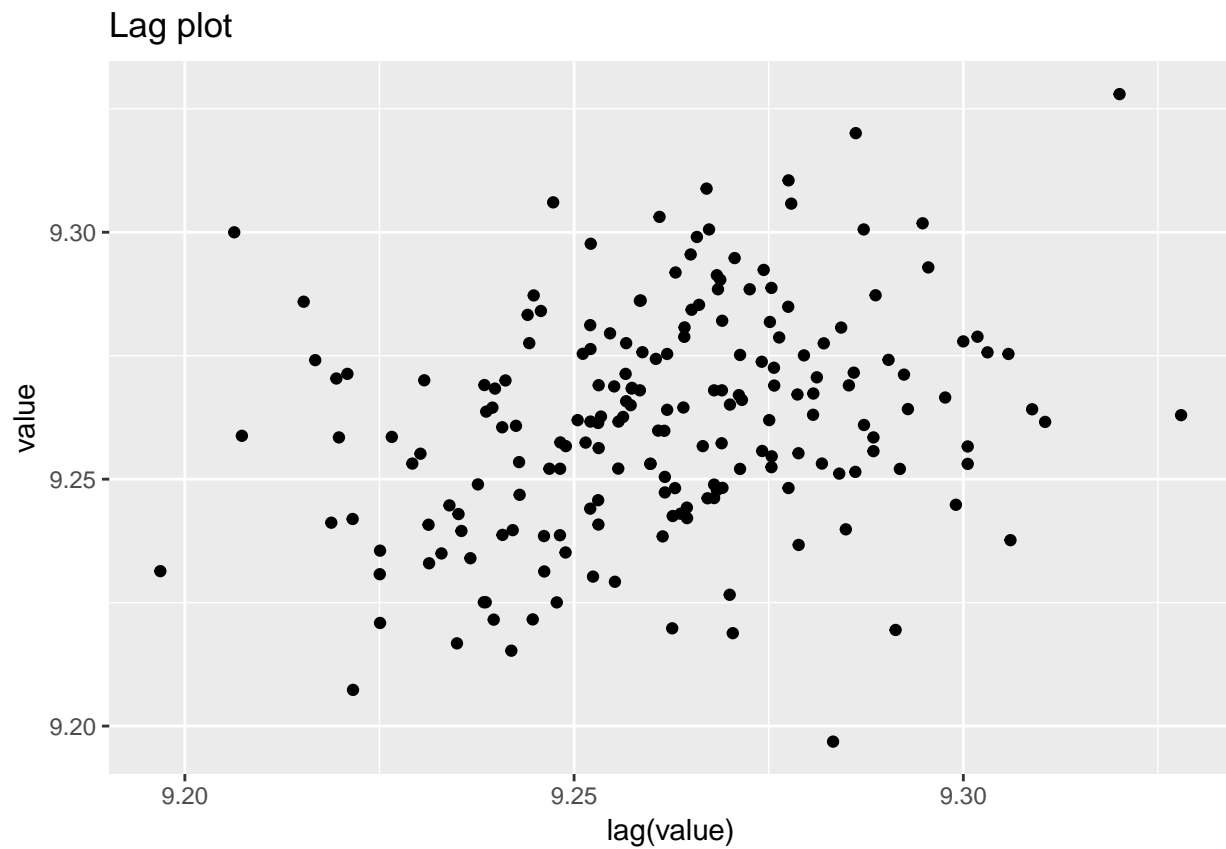
```
ggplot(heat_flow_meter1, aes(rowid, value)) +
  geom_line() +
```

```
labs(title = "Run sequence plot")
```



```
ggplot(heat_flow_meter1, aes(lag(value), value)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

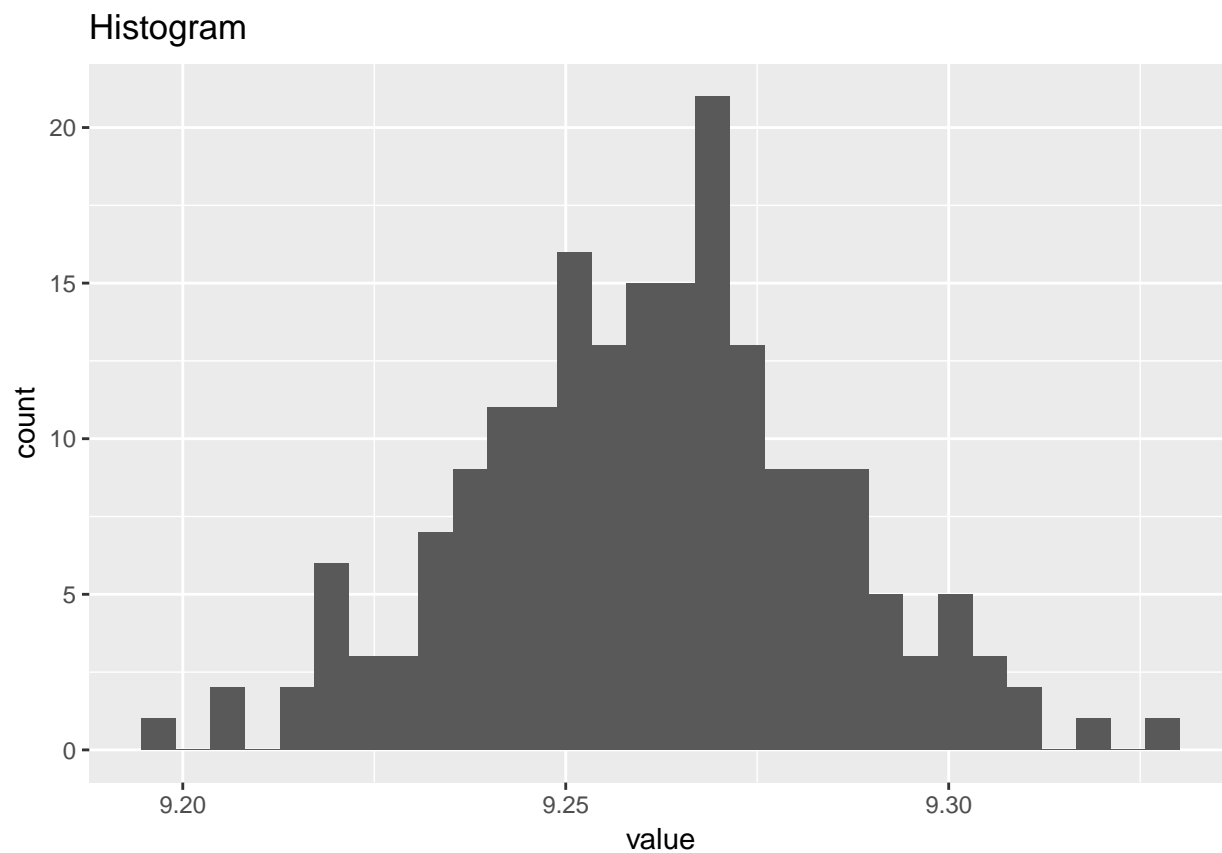
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



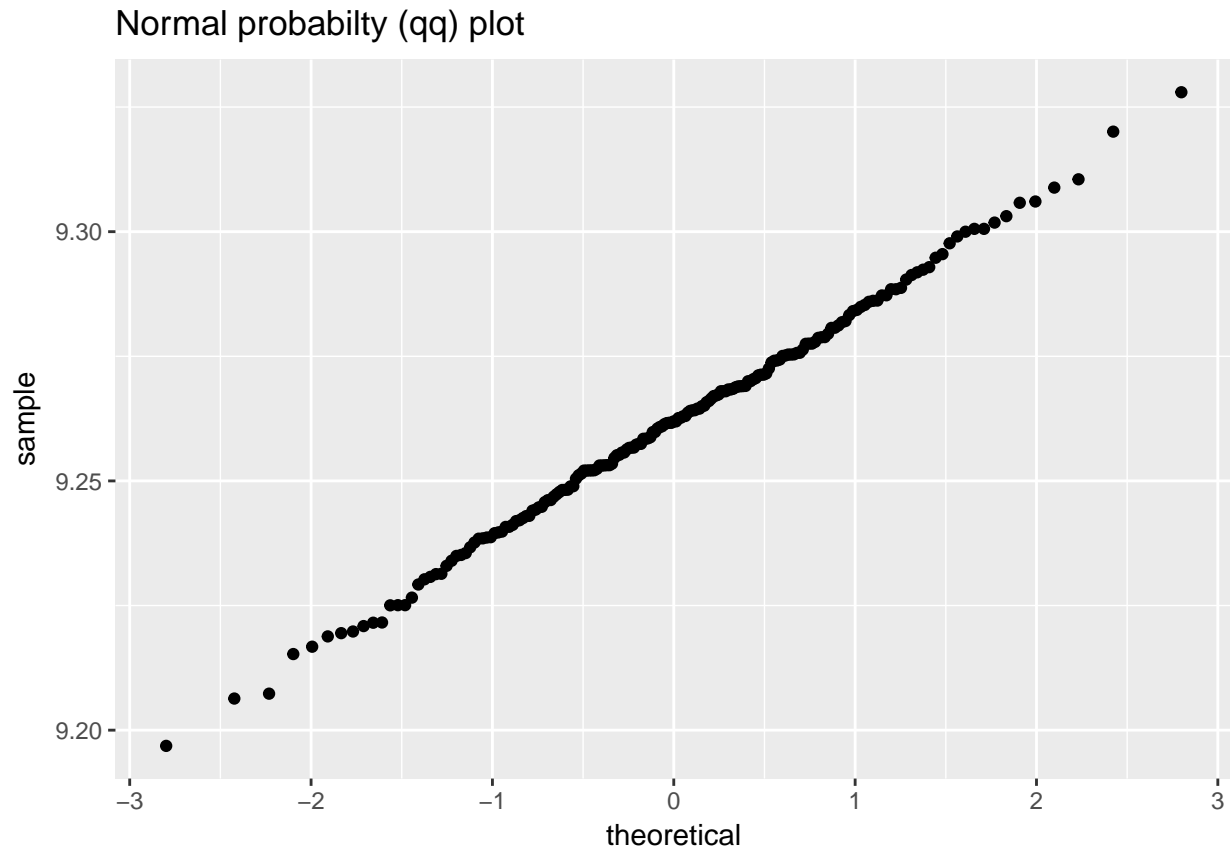
```
ggplot(heat_flow_meter1, aes(value)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```





```
ggplot(heat_flow_meter1, aes(sample = value)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



### 1.4.8 Ceramic strength

Ceramic Strength

```
ceramic_strength <- read_table2("NIST data/JAHANMI2.DAT", skip = 48, col_names = TRUE) %>%
  filter(Lab >= 1) %>%
  rowid_to_column()
```

```
## Parsed with column specification:
```

```
## cols(
##   Id = col_character(),
##   Lab = col_integer(),
##   Num = col_integer(),
##   Test = col_integer(),
##   Y = col_double(),
##   X1 = col_integer(),
##   X2 = col_integer(),
##   X3 = col_integer(),
##   X4 = col_integer(),
##   Trt = col_integer(),
##   Set = col_integer(),
##   Llab = col_double(),
##   Rep = col_integer(),
##   Bat = col_integer(),
##   Sblab = col_double(),
##   Set2 = col_integer()
```

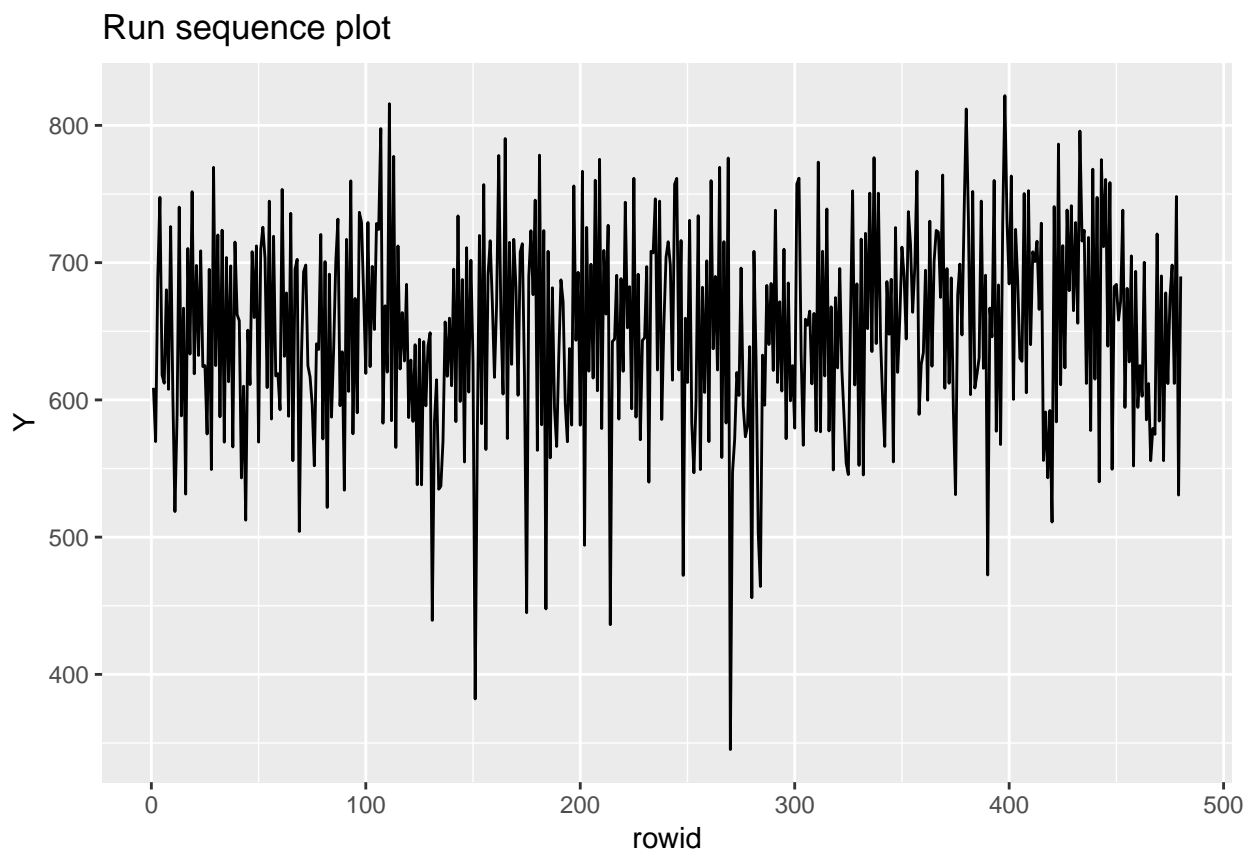
```
## )

## Warning in rbind(names(probs), probs_f): number of columns of result is not
## a multiple of vector length (arg 2)

## Warning: 1 parsing failure.
## row # A tibble: 1 x 5 col      row col      expected      actual      file      expected      <in>
ceramic_strength

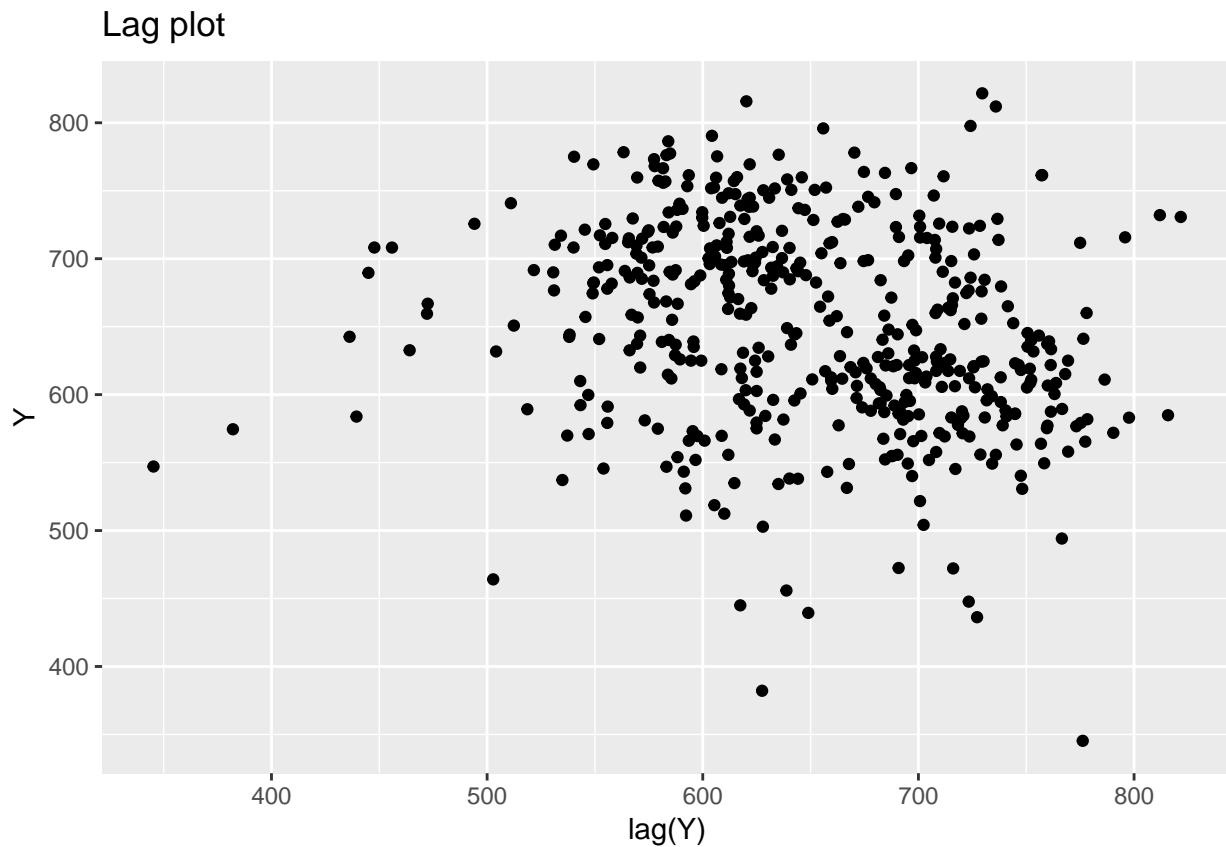
## # A tibble: 480 x 17
##   rowid Id      Lab  Num  Test      Y      X1      X2      X3      X4      Trt      Set
##   <int> <chr> <int> <int> <int> <dbl> <int> <int> <int> <int> <int> <int>
## 1     1 1 1      1     1     609.    -1    -1    -1    -1     1     1
## 2     2 2 2      1     2     570.    -1    -1    -1    -1     1     1
## 3     3 3 3      1     3     690.    -1    -1    -1    -1     1     1
## 4     4 4 4      1     4     748.    -1    -1    -1    -1     1     1
## 5     5 5 5      1     5     618.    -1    -1    -1    -1     1     1
## 6     6 6 6      1     6     612.    -1    -1    -1    -1     1     1
## 7     7 7 7      1     7     680.    -1    -1    -1    -1     1     1
## 8     8 8 8      1     8     608.    -1    -1    -1    -1     1     1
## 9     9 9 9      1     9     726.    -1    -1    -1    -1     1     1
## 10    10 10 10     1    10     605.    -1    -1    -1    -1     1     1
## # ... with 470 more rows, and 5 more variables: Llab <dbl>, Rep <int>,
## #   Bat <int>, Sblab <dbl>, Set2 <int>

ggplot(ceramic_strength, aes(rowid, Y)) +
  geom_line() +
  labs(title = "Run sequence plot")
```



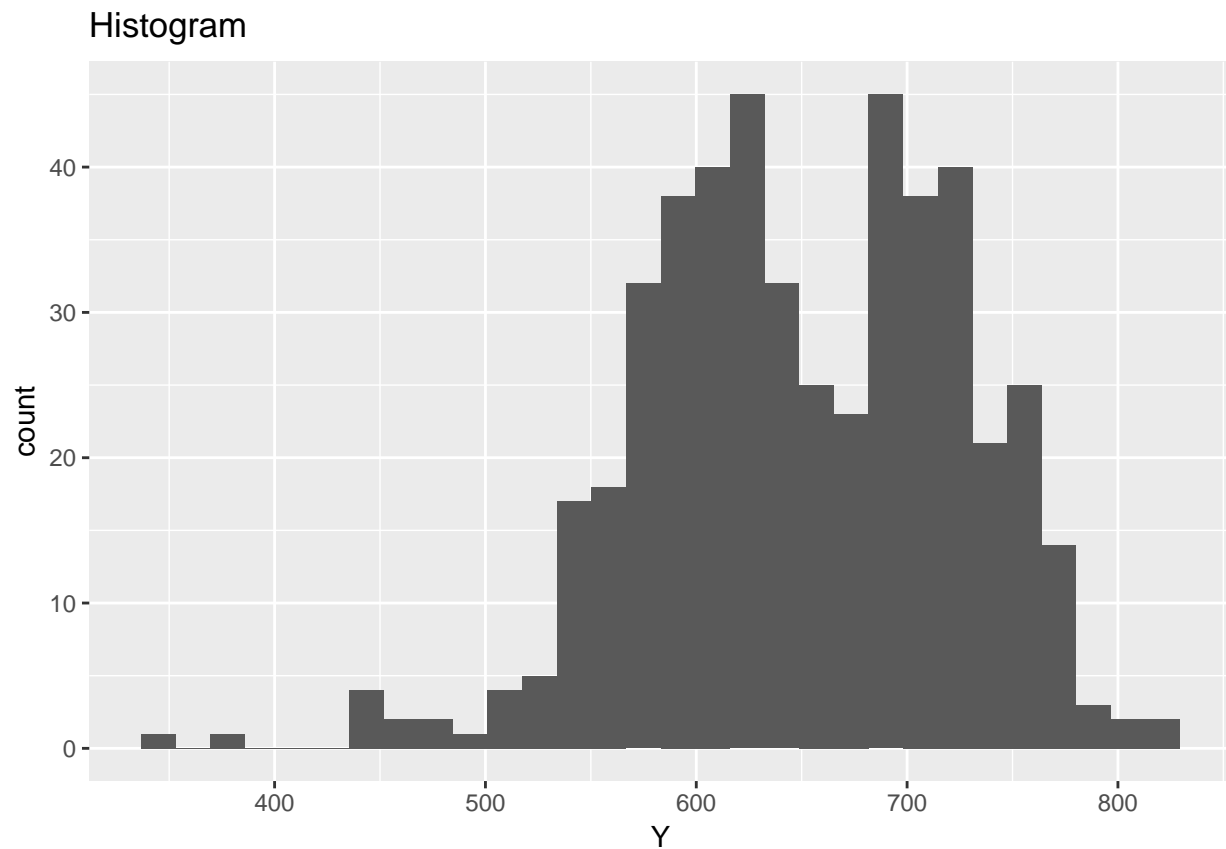
```
ggplot(ceramic_strength, aes(lag(Y), Y)) +  
  geom_point() +  
  labs(title = "Lag plot")
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

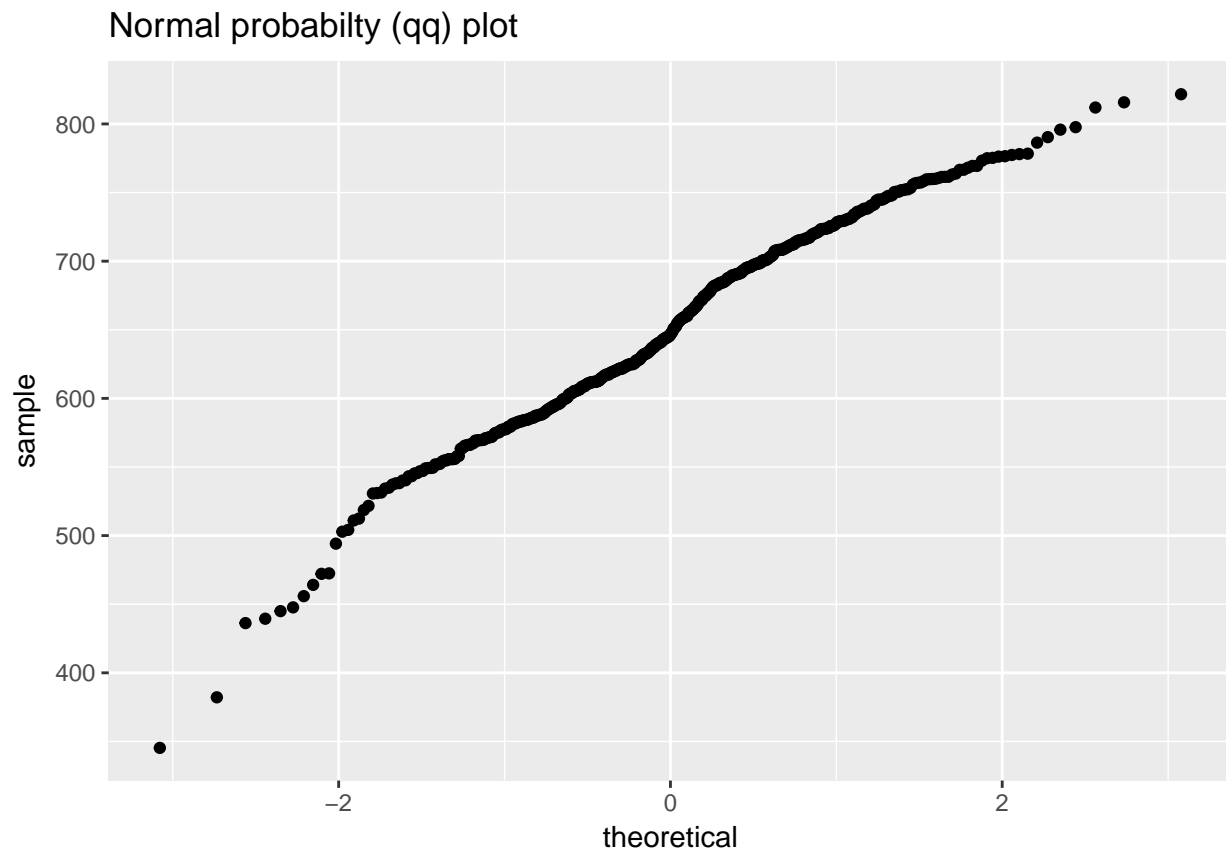


```
ggplot(ceramic_strength, aes(Y)) +  
  geom_histogram() +  
  labs(title = "Histogram")
```

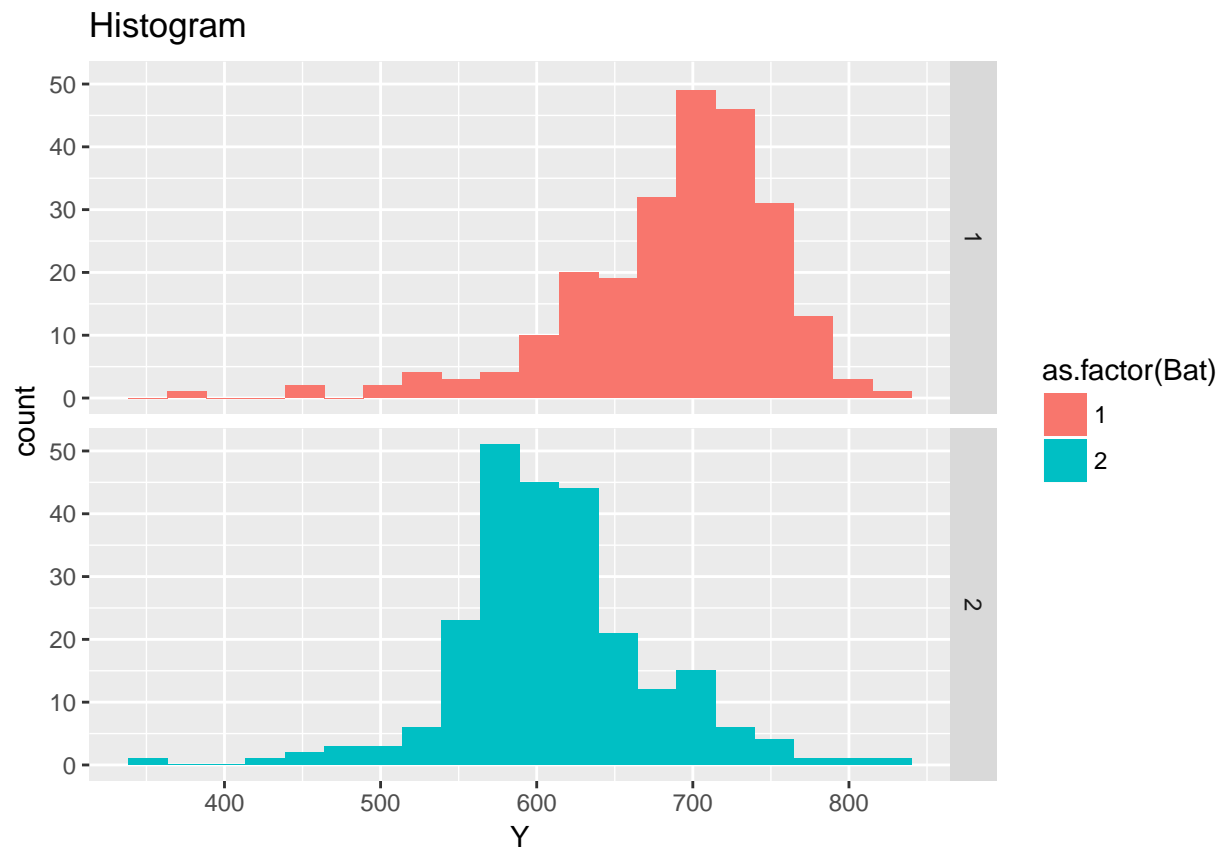
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



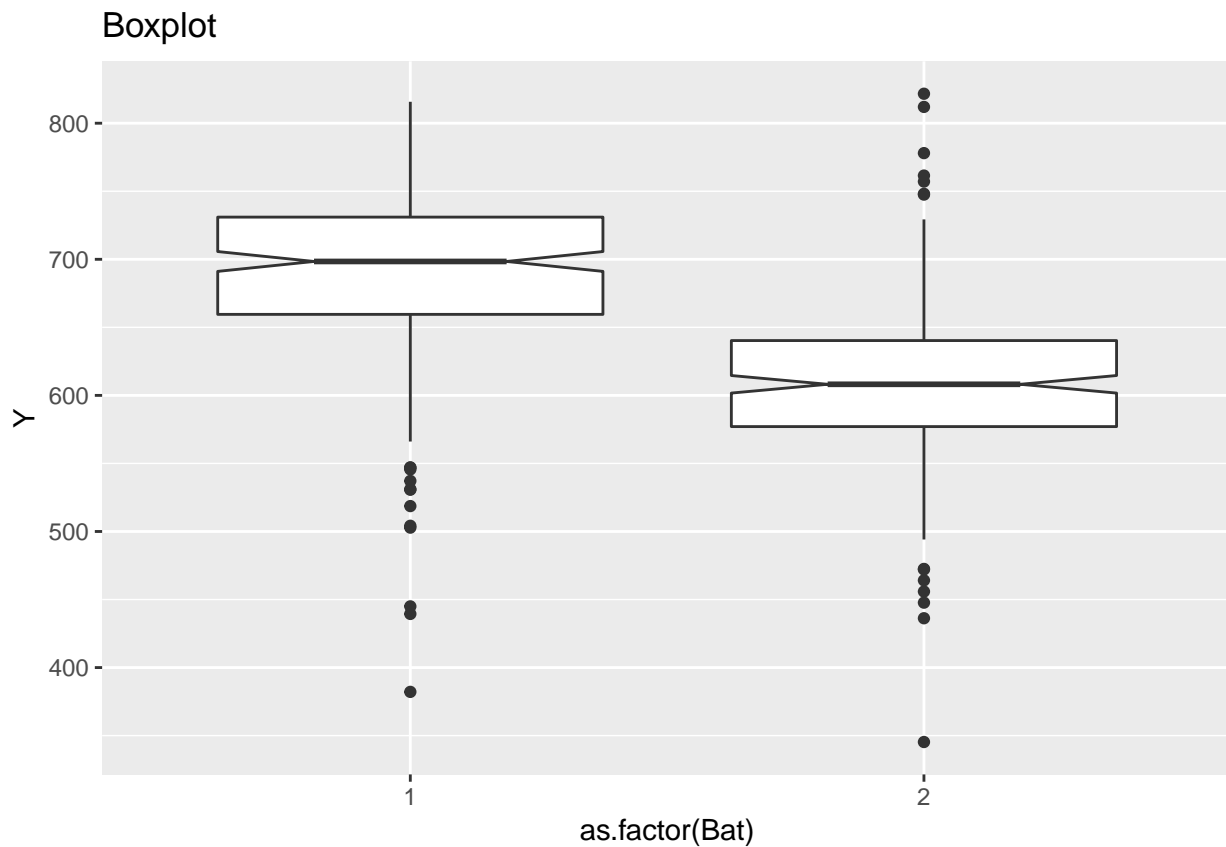
```
ggplot(ceramic_strength, aes(sample = Y)) +  
  geom_qq() +  
  labs(title = "Normal probabiltiy (qq) plot")
```



```
ggplot(ceramic_strength, aes(Y)) +  
  geom_histogram(aes(fill = as.factor(Bat)), bins = 20) +  
  facet_grid(Bat ~ .) +  
  labs(title = "Histogram")
```

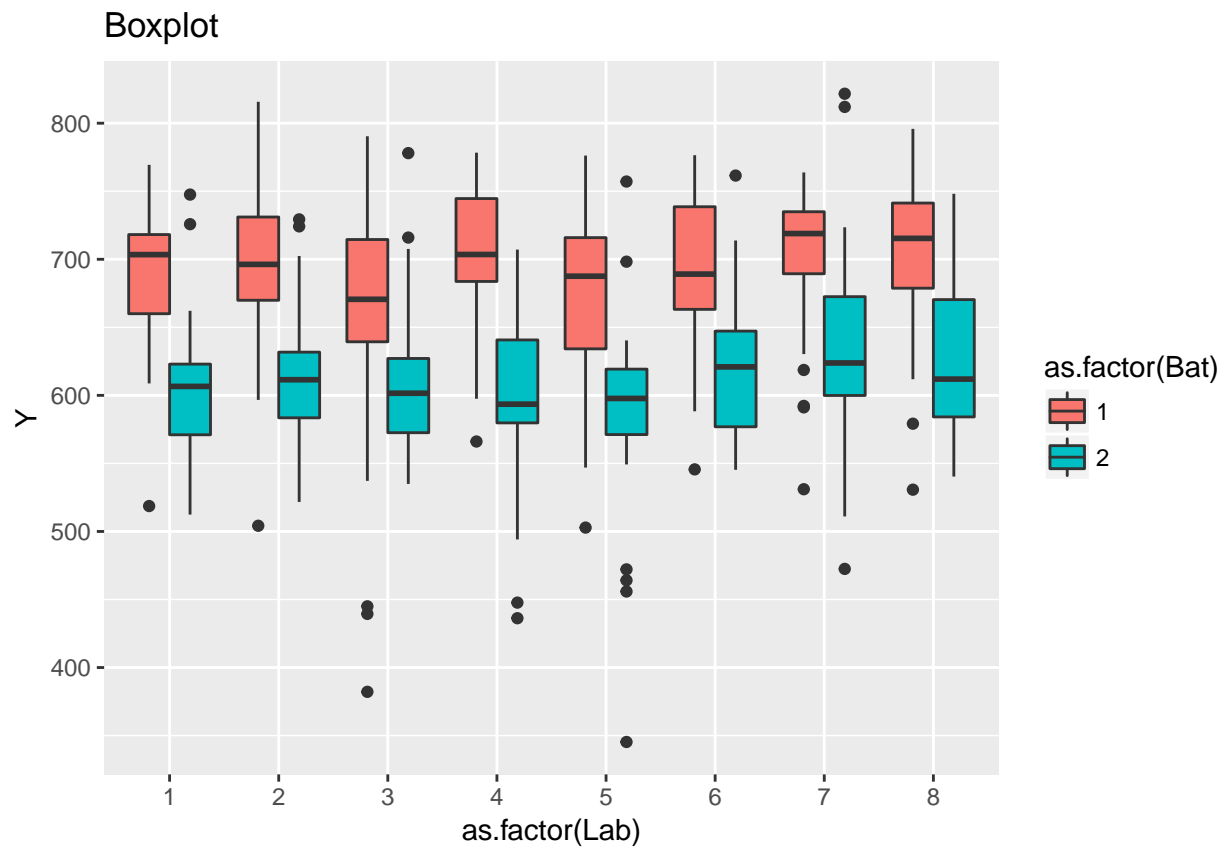


```
ggplot(ceramic_strength, aes(as.factor(Bat), Y)) +  
  geom_boxplot(notch = TRUE) +  
  labs(title = "Boxplot")
```



```
ggplot(ceramic_strength, aes(as.factor(Lab), Y)) +  
  geom_boxplot(aes(fill = as.factor(Bat))) +  
  labs(title = "Boxplot")
```







## Chapter 2

# Measurement Process Characterization

### 2.1 Packages used in this chapter

```
library(magrittr)
library(tidyverse)
```

### 2.2 Characterization

### 2.3 Gauge R & R studies

### 2.4 Case Studies

#### 2.4.1 Check standard

##### 2.4.1.1 Background and data

The measurements on the check standard duplicate certification measurements that were being made, during the same time period, on individual wafers from crystal #51939. For the check standard there were:

- J = 6 repetitions at the center of the wafer on each day
- K = 25 days

Check standard for resistivity measurement

##### 2.4.1.2 Reading the dataset

```
check_standard <- read_table2("NIST data/MPC62_clean.DAT", col_names = TRUE) %>%
  rowid_to_column()
```

```
## Parsed with column specification:
## cols(
##   Crystal_ID = col_integer(),
##   Wafer_ID = col_integer(),
##   Month = col_character(),
##   Day = col_character(),
##   Hour = col_character(),
##   Minute = col_character(),
##   Operator = col_integer(),
##   Humidity = col_integer(),
##   Probe_ID = col_integer(),
##   Temperature = col_double(),
##   Resistance = col_double(),
##   Stdev = col_double(),
##   Df = col_integer()
## )
```

```
check_standard
```

```
## # A tibble: 25 x 14
##   rowid Crystal_ID Wafer_ID Month Day   Hour Minute Operator Humidity
##   <int>   <int>     <int> <chr> <chr> <chr> <chr>   <int>   <int>
## 1     1       51939     137 03   24   18    01         1     42
## 2     2       51939     137 03   25   12    41         1     35
## 3     3       51939     137 03   25   15    57         1     33
## 4     4       51939     137 03   28   10    10         2     47
## 5     5       51939     137 03   28   13    31         2     44
## 6     6       51939     137 03   28   17    33         1     43
## 7     7       51939     137 03   29   14    40         1     36
## 8     8       51939     137 03   29   16    33         1     35
## 9     9       51939     137 03   30   05    45         2     32
## 10    10       51939     137 03   30   09    26         2     33
## # ... with 15 more rows, and 5 more variables: Probe_ID <int>,
## #   Temperature <dbl>, Resistance <dbl>, Stdev <dbl>, Df <int>
```

### 2.4.1.3 Level-1 standard deviation

Measurements for  $J$  runs over  $K$  days for  $L$  runs are:

$$Y_{lkj}(l = 1, \dots, L, k = 1, \dots, K, j = 1, \dots, J)$$

The level-1 repeatability (short term precision) is calculated from the pooled standard deviation over days and runs

$$s_{1lk} = \sqrt{\frac{1}{J-1} \sum_{j=1}^J (Y_{lkj} - \bar{Y}_{lk\bullet})^2}$$

with

$$\bar{Y}_{lk\bullet} = \frac{1}{J} \sum_{j=1}^J \bar{Y}_{lkj}$$

As stated in the e-Handbook: >An individual short-term standard deviation will not be a reliable estimate of precision if the degrees of freedom is less than ten, but the individual estimates can be pooled over the K days to obtain a more reliable estimate.

The pooled level-1 standard deviation estimate with  $v = K(J - 1)$  degrees of freedom is

$$s_1 = \sqrt{\frac{1}{K} \sum_{k=1}^K s_k^2}$$

```
s1_chkstd <- check_standard %>%
  mutate(Stdev_sq = Stdev^2) %$%
  mean(Stdev_sq) %>%
  sqrt()
```

```
s1_chkstd
```

```
## [1] 0.06138795
```

Several comments on the code above. I've introduced the `%$%` operator. This allows me to use individual columns from my data frame and is useful for performing mathematical operations on a specific column of data. It is from the **magrittr** package.

I find this type of code easy to read and understand. Describing the operations is simple, I'm just working from inside out of the equation:

- creating a new column of data that is  $(Stdev)^2$
- finding the mean of that new column
- taking the square root of that number to give  $s_1$ .

#### 2.4.1.4 Level-2 standard deviation (reproducibility)

$$s_{chkstd} = s_2 = \sqrt{\frac{1}{K-1} \sum_{k=1}^K (\bar{Y}_{k\bullet} - \bar{Y}_{\bullet\bullet})^2}$$

with

$$\bar{Y}_{\bullet\bullet} = \frac{1}{K} \sum_{k=1}^K \bar{Y}_{k\bullet}$$

Which is simply the standard deviation of the daily measurements

```
s2_chkstd <- check_standard %$%
  sd(Resistance)
```

```
s2_chkstd
```

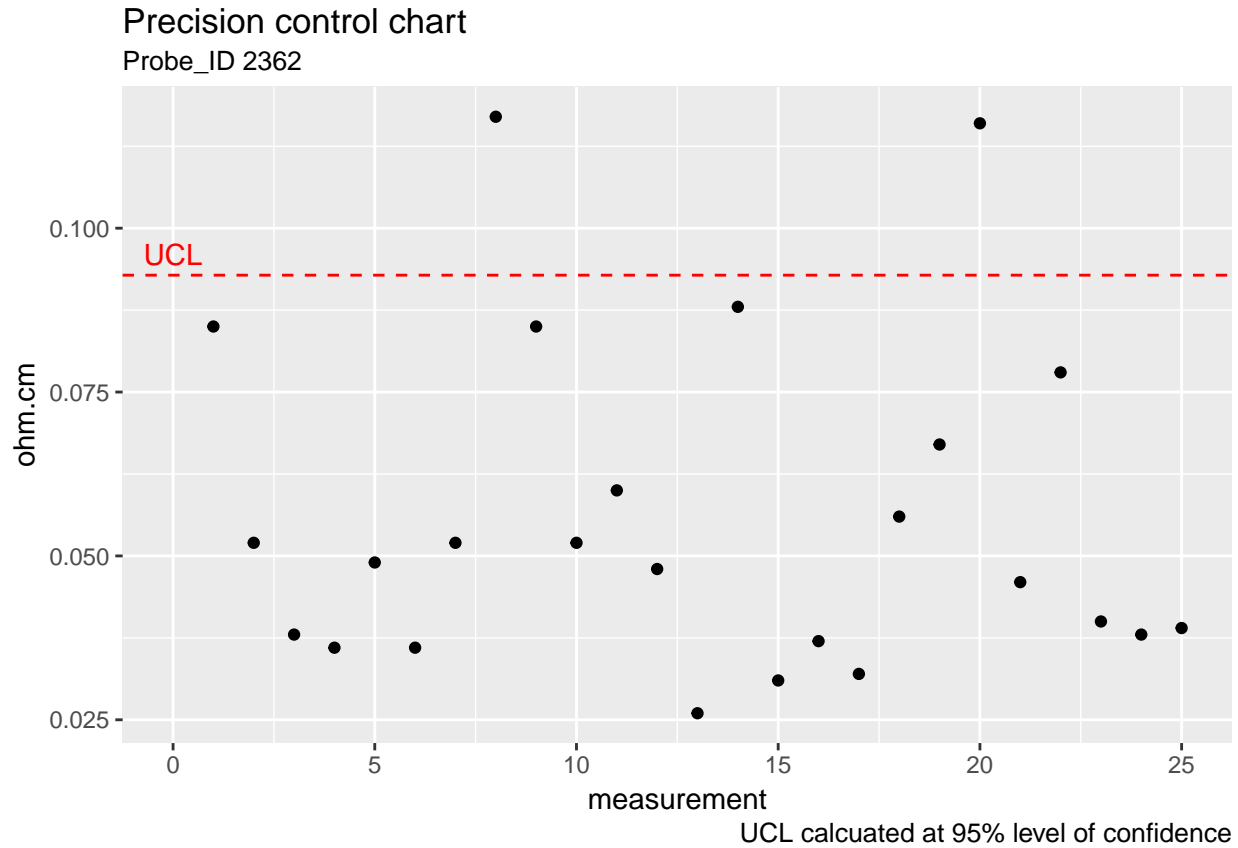
```
## [1] 0.02679813
```

#### 2.4.1.5 Control chart for standard deviation - Precision

```
UCL_precision_ckkstd <- s1_chkstd*sqrt(qf(0.95, 5, 125))
UCL_precision_ckkstd
```

```
## [1] 0.0928313
```

```
ggplot(check_standard) +
  geom_point(aes(rowid, Stdev)) +
  geom_hline(aes(yintercept = UCL_precision_ckkstd), colour = "red", linetype = "dashed") +
  labs(title = "Precision control chart", subtitle = "Probe_ID 2362", x = "measurement", y = "ohm.cm") +
  annotate("text", x = 0, y = 0.096, label = "UCL", colour = "red")
```

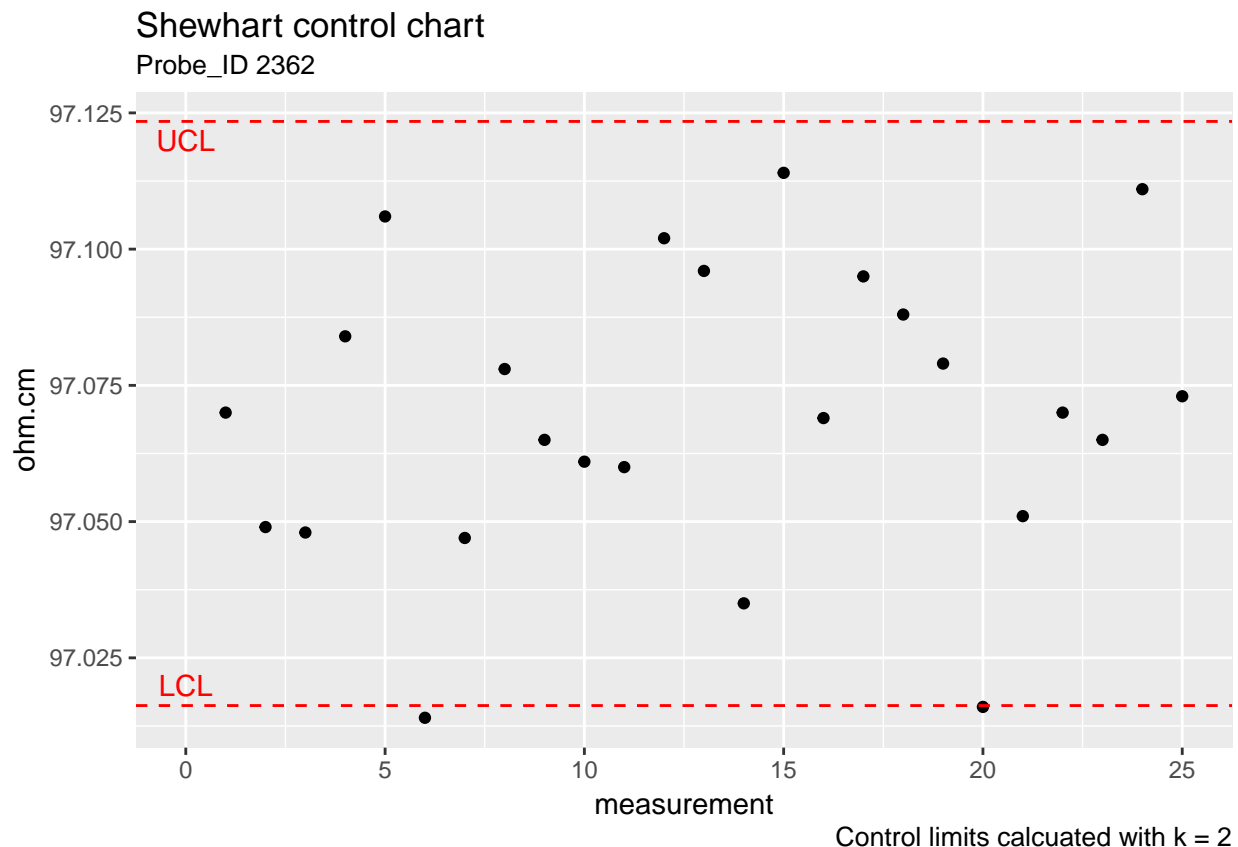


#### 2.4.1.6 Control chart for measurement bias and variability

The control limits for monitoring the bias and long-term variability of resistivity with a Shewhart control chart are given by

$$UCL = \text{Average} + 2 \cdot s_2 \text{Centerline} = \text{Average} LCL = \text{Average} - 2 \cdot s_2$$

```
ggplot(check_standard) +
  geom_point(aes(rowid, Resistance)) +
  geom_hline(aes(yintercept = (mean(Resistance) + 2*s2_chkstd)), colour = "red", linetype = "dashed") +
  geom_hline(aes(yintercept = (mean(Resistance) - 2*s2_chkstd)), colour = "red", linetype = "dashed") +
  labs(title = "Shewhart control chart", subtitle = "Probe_ID 2362", x = "measurement", y = "ohm.cm") +
  annotate("text", x = 0, y = 97.12, label = "UCL", colour = "red") +
  annotate("text", x = 0, y = 97.02, label = "LCL", colour = "red")
```



## 2.4.2 Gauge study

### 2.4.2.1 Background and data

Measurements on the check standards are used to estimate repeatability, day effect, and run effect. The effect of operator was not considered to be significant for this study; therefore, 'day' replaces 'operator' as a factor in the nested design. Averages and standard deviations from  $J = 6$  measurements at the center of each wafer are shown in the table.

- $J = 6$  measurements at the center of the wafer per day
- $K = 6$  days (one operator) per repetition
- $L = 2$  runs (complete)
- $Q = 5$  wafers (check standards 138, 139, 140, 141, 142)
- $R = 5$  probes (1, 281, 283, 2062, 2362)

Gauge study of resistivity probes

```
gauge_study <- read_table2("NIST data/MPC61_clean.DAT", col_names = TRUE) %>%
  rowid_to_column()
```

```
## Parsed with column specification:
## cols(
##   RUN = col_integer(),
##   WAFER = col_double(),
##   PROBE = col_double(),
##   MONTH = col_double(),
##   DAY = col_double(),
```

```
## OP = col_double(),
## TEMP = col_double(),
## AVERAGE = col_double(),
## STDDEV = col_double()
## )
```

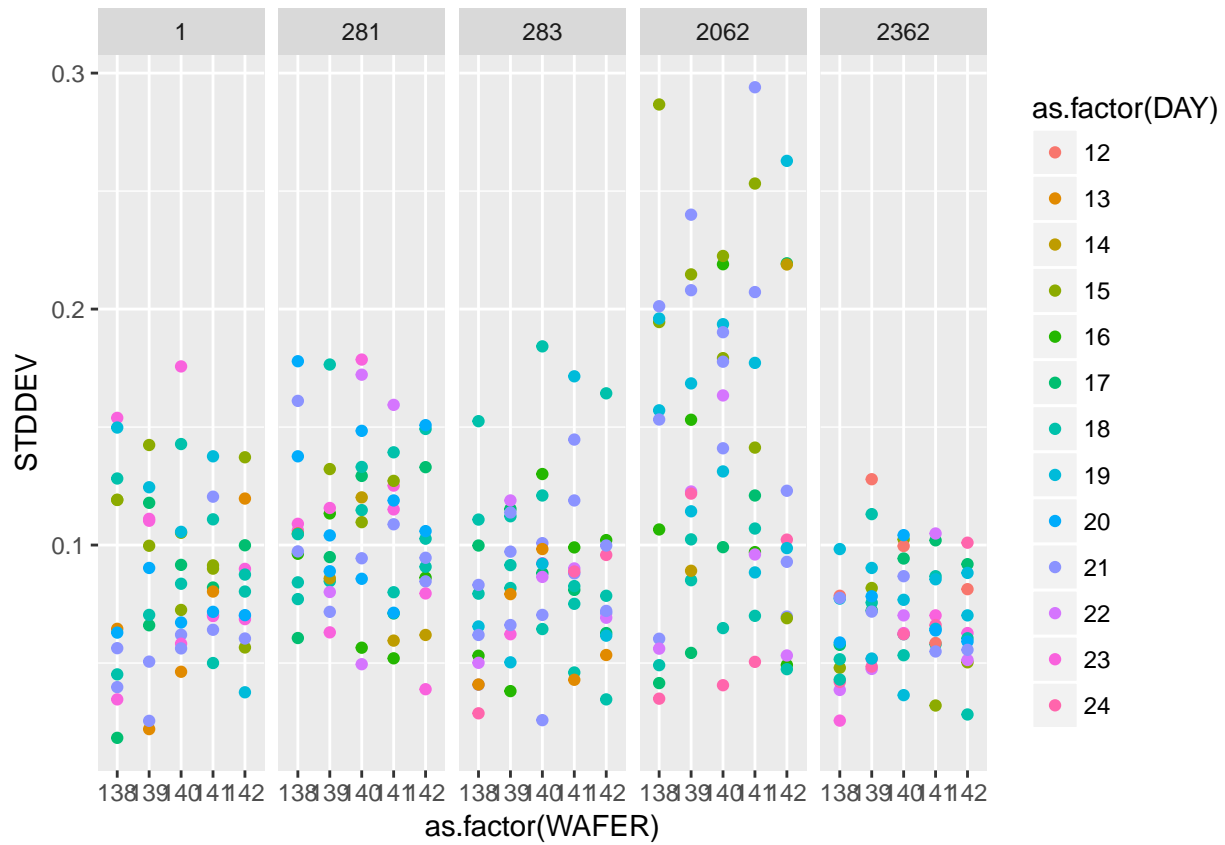
```
gauge_study
```

```
## # A tibble: 300 x 10
##   rowid  RUN WAFER PROBE MONTH  DAY    OP  TEMP AVERAGE STDDEV
##   <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>   <dbl>  <dbl>
## 1     1     1     1  138.    1.    3.   15.    1.   23.0    95.2  0.119
## 2     2     2     1  138.    1.    3.   17.    1.   23.0    95.2  0.0183
## 3     3     3     1  138.    1.    3.   18.    1.   22.8    95.2  0.128
## 4     4     4     1  138.    1.    3.   21.    1.   23.2    95.2  0.0398
## 5     5     5     1  138.    1.    3.   23.    2.   23.2    95.1  0.0346
## 6     6     6     1  138.    1.    3.   23.    1.   23.2    95.1  0.154
## 7     7     7     1  138.  281.    3.   16.    1.   23.0    95.2  0.0963
## 8     8     8     1  138.  281.    3.   17.    1.   23.0    95.1  0.0606
## 9     9     9     1  138.  281.    3.   18.    1.   22.8    95.1  0.0842
## 10    10    10     1  138.  281.    3.   21.    1.   23.3    95.1  0.0973
## # ... with 290 more rows
```

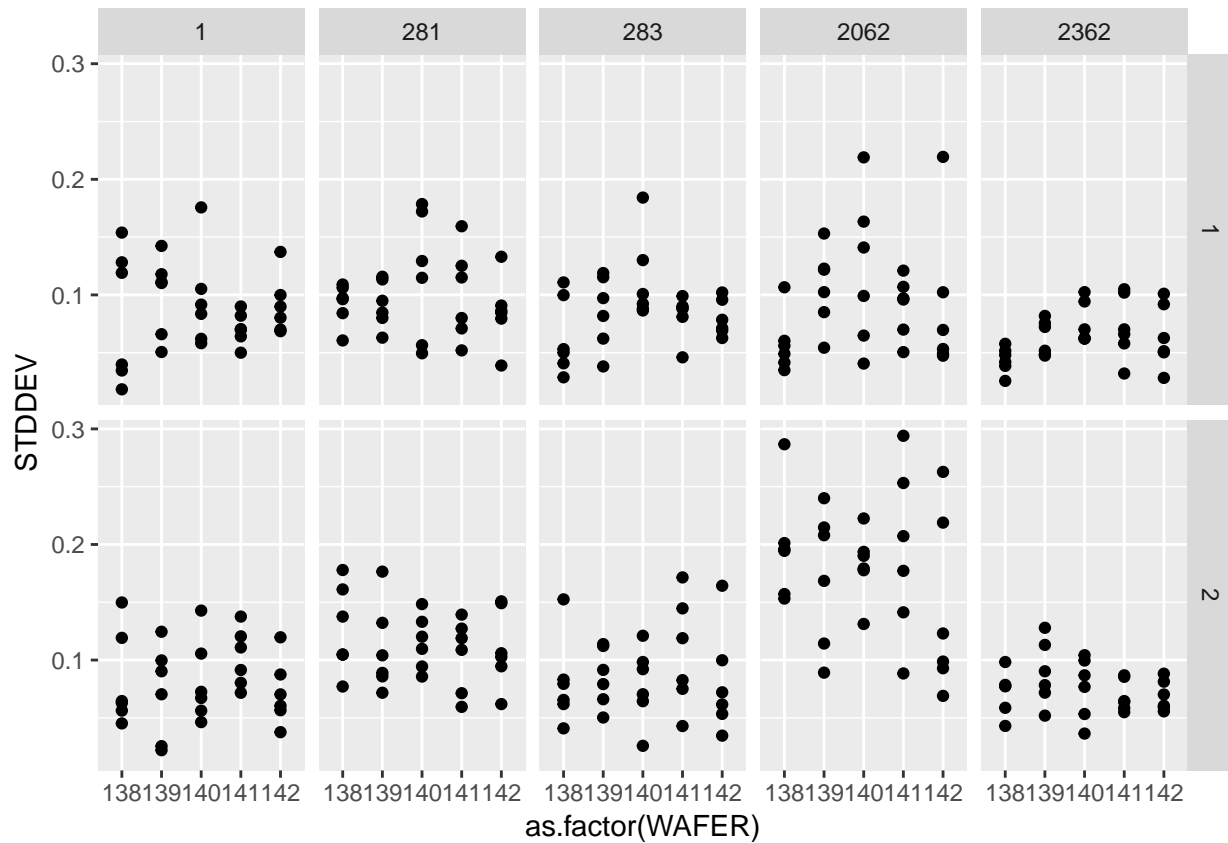
#### 2.4.2.2 Repeatability standard deviations

```
ggplot(gauge_study) +
  geom_point(aes(as.factor(WAFER), STDDEV, colour = as.factor(DAY))) +
  facet_wrap(~ as.factor(PROBE), nrow = 1)
```



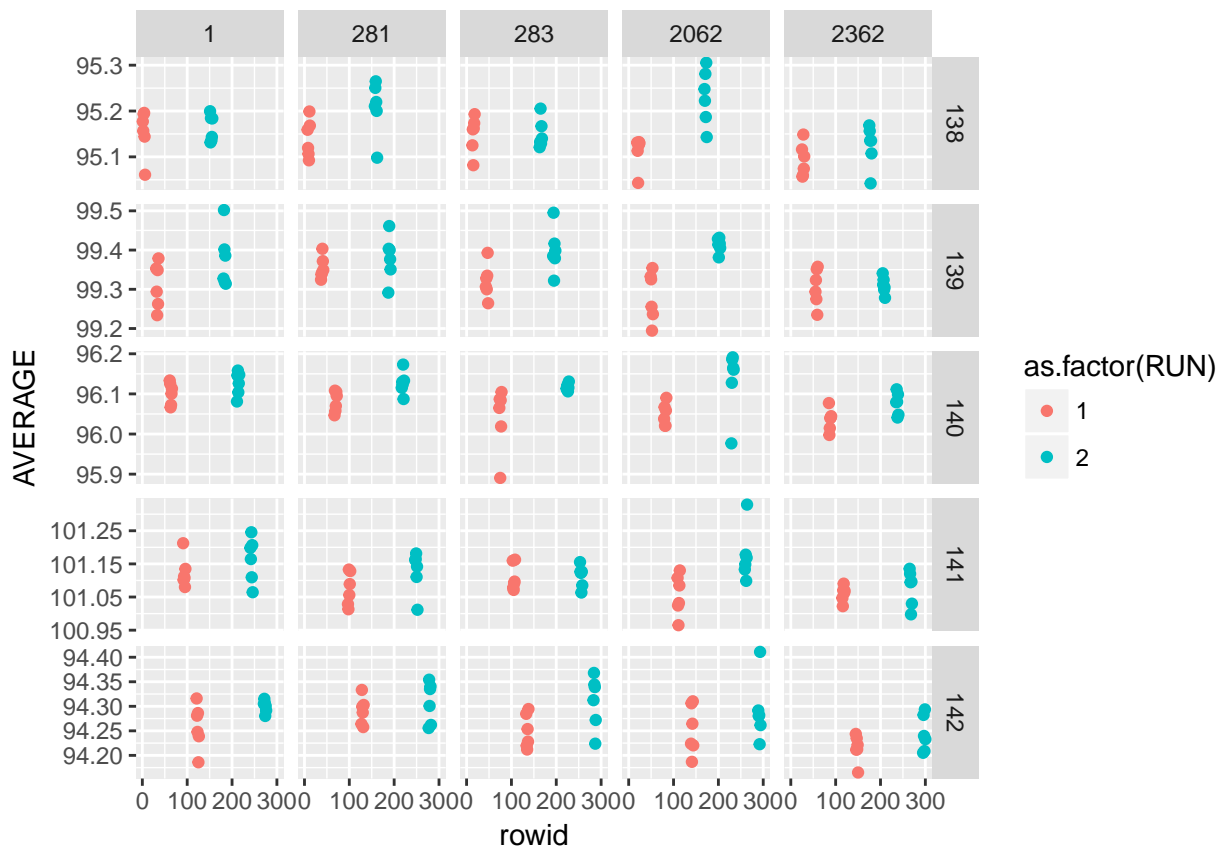


```
ggplot(gauge_study) +
  geom_point(aes(as.factor(WAFER), STDDEV)) +
  facet_grid(as.factor(RUN) ~ as.factor(PROBE))
```



### 2.4.2.3 Effects of days and long-term stability

```
ggplot(gauge_study) +
  geom_point(aes(rowid, AVERAGE, colour = as.factor(RUN))) +
  facet_grid(as.factor(WAFER) ~ as.factor(PROBE), scales = "free_y")
```



#### 2.4.2.4 Differences among 5 probes

```
probe_means_run <- gauge_study %>%
  group_by(PROBE, WAFER, RUN) %>%
  summarise(n = n(), probe_mean = mean(AVERAGE)) %>%
  unite(join_id, WAFER, RUN, sep = "_", remove = FALSE) %>%
  ungroup()
```

```
probe_means_run
```

```
## # A tibble: 50 x 6
##   PROBE join_id WAFER  RUN      n probe_mean
##   <dbl> <chr>   <dbl> <int> <int>   <dbl>
## 1 1. 138_1 138.     1     6     95.2
## 2 1. 138_2 138.     2     6     95.2
## 3 1. 139_1 139.     1     6     99.3
## 4 1. 139_2 139.     2     6     99.4
## 5 1. 140_1 140.     1     6     96.1
## 6 1. 140_2 140.     2     6     96.1
## 7 1. 141_1 141.     1     6    101.
## 8 1. 141_2 141.     2     6    101.
## 9 1. 142_1 142.     1     6     94.3
##10 1. 142_2 142.     2     6     94.3
## # ... with 40 more rows
```

```

wafer_means_run <- gauge_study %>%
  group_by(WAFER, RUN) %>%
  summarise(n = n(), wafer_means = mean(AVERAGE)) %>%
  unite(join_id, WAFER, RUN, sep = "_", remove = FALSE) %>%
  ungroup()

wafer_means_run

```

```

## # A tibble: 10 x 5
##   join_id WAFER  RUN      n wafer_means
##   <chr>   <dbl> <int> <int>      <dbl>
## 1 138_1    138.     1    30      95.1
## 2 138_2    138.     2    30      95.2
## 3 139_1    139.     1    30      99.3
## 4 139_2    139.     2    30      99.4
## 5 140_1    140.     1    30      96.1
## 6 140_2    140.     2    30      96.1
## 7 141_1    141.     1    30     101.
## 8 141_2    141.     2    30     101.
## 9 142_1    142.     1    30      94.3
## 10 142_2    142.     2    30      94.3

```

```

delta_probes <- left_join(probe_means_run, wafer_means_run, by = "join_id") %>%
  mutate(delta_probes_wafer = probe_mean - wafer_means)

delta_probes

```

```

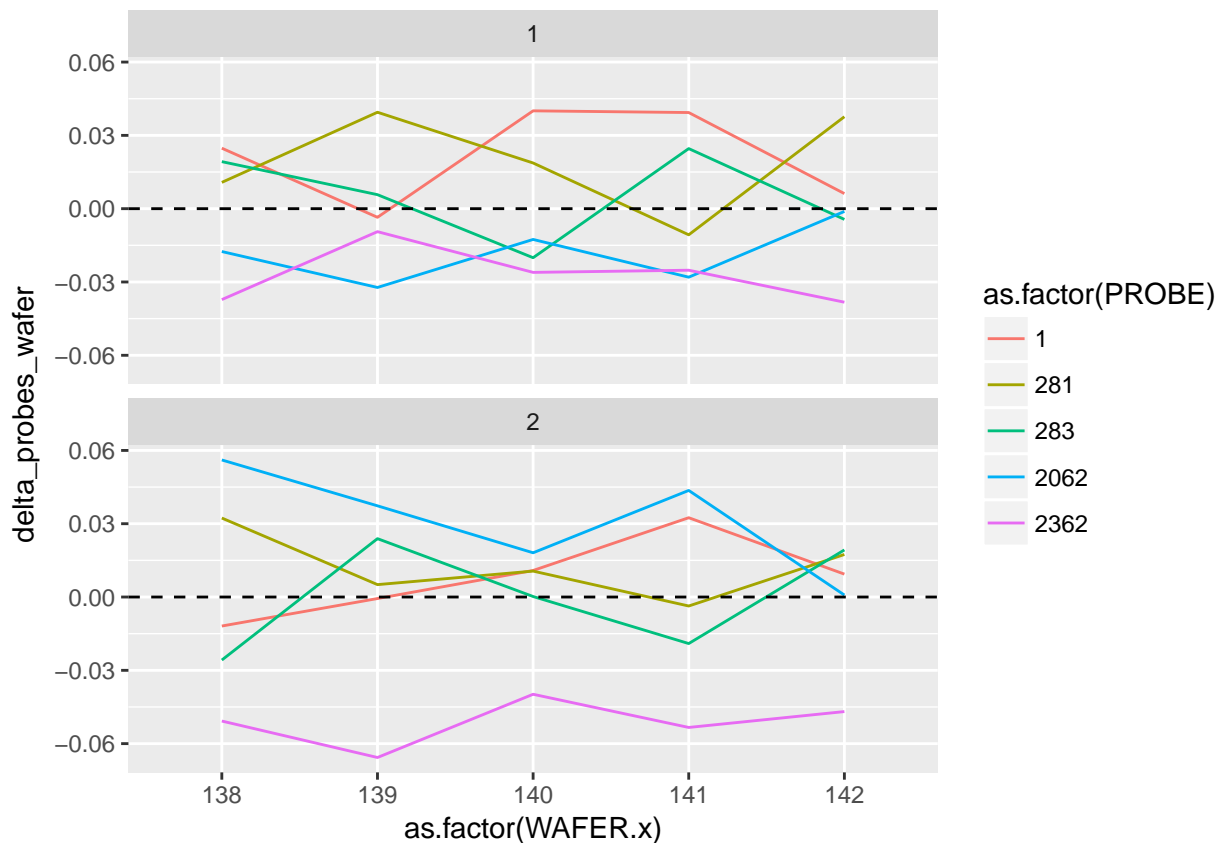
## # A tibble: 50 x 11
##   PROBE join_id WAFER.x RUN.x   n.x probe_mean WAFER.y RUN.y   n.y
##   <dbl> <chr>   <dbl> <int> <int>      <dbl>   <dbl> <int> <int>
## 1 1. 138_1    138.     1     6      95.2    138.     1     30
## 2 1. 138_2    138.     2     6      95.2    138.     2     30
## 3 1. 139_1    139.     1     6      99.3    139.     1     30
## 4 1. 139_2    139.     2     6      99.4    139.     2     30
## 5 1. 140_1    140.     1     6      96.1    140.     1     30
## 6 1. 140_2    140.     2     6      96.1    140.     2     30
## 7 1. 141_1    141.     1     6     101.    141.     1     30
## 8 1. 141_2    141.     2     6     101.    141.     2     30
## 9 1. 142_1    142.     1     6      94.3    142.     1     30
## 10 1. 142_2    142.     2     6      94.3    142.     2     30
## # ... with 40 more rows, and 2 more variables: wafer_means <dbl>,
## #   delta_probes_wafer <dbl>

```

```

ggplot(delta_probes) +
  geom_line(aes(as.factor(WAFER.x), delta_probes_wafer, group = as.factor(PROBE), colour = as.factor(PROBE)),
  geom_hline(aes(yintercept = 0), linetype = "dashed") +
  facet_wrap(~ as.factor(RUN.x), ncol = 1)

```



#### 2.4.2.5 Analysis and interpretation

Table of estimates for probe #2362

A graphical analysis shows repeatability standard deviations plotted by wafer and probe... The plots show that for both runs the precision of this probe is better than for the other probes.

Probe #2362, because of its superior precision, was chosen as the tool for measuring all 100 ohm.cm resistivity wafers at NIST. Therefore, the remainder of the analysis focuses on this probe.

#### 2.4.2.6 probe #2362

```
probe_2362 <- gauge_study %>%
  filter(PROBE == 2362)
```

```
probe_2362
```

```
## # A tibble: 60 x 10
```

```
##   rowid  RUN WAFER PROBE MONTH  DAY  OP  TEMP AVERAGE STDDEV
##   <int> <int> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>   <dbl>  <dbl>
## 1    25    1  138. 2362.    3.   15.   1.  23.1    95.1 0.0480
## 2    26    1  138. 2362.    3.   17.   1.  23.0    95.1 0.0577
## 3    27    1  138. 2362.    3.   18.   1.  23.0    95.1 0.0516
## 4    28    1  138. 2362.    3.   22.   1.  23.2    95.1 0.0386
## 5    29    1  138. 2362.    3.   23.   2.  23.3    95.1 0.0256
```

```
## 6      30      1 138. 2362.      3. 24.      2. 23.1      95.1 0.0420
## 7      55      1 139. 2362.      3. 15.      1. 23.1      99.3 0.0818
## 8      56      1 139. 2362.      3. 17.      1. 23.0      99.3 0.0723
## 9      57      1 139. 2362.      3. 18.      1. 22.9      99.3 0.0756
## 10     58      1 139. 2362.      3. 22.      1. 23.3      99.4 0.0475
## # ... with 50 more rows
```

Pooled level-1 standard deviations (ohm.cm)

```
s1_2362_1 <- probe_2362 %>%
  filter(RUN == 1) %>%
  mutate(Stdev_sq = STDDEV^2) %$%
  mean(Stdev_sq) %>%
  sqrt()
```

```
s1_2362_1
```

```
## [1] 0.06750898
```

```
s1_2362_2 <- probe_2362 %>%
  filter(RUN == 2) %>%
  mutate(Stdev_sq = STDDEV^2) %$%
  mean(Stdev_sq) %>%
  sqrt()
```

```
s1_2362_2
```

```
## [1] 0.07785664
```

```
s1_2362 <- probe_2362 %>%
  mutate(Stdev_sq = STDDEV^2) %$%
  mean(Stdev_sq) %>%
  sqrt()
```

```
s1_2362
```

```
## [1] 0.07286673
```

Level-2 standard deviations (ohm.cm) for 5 wafers

```
s2_2362 <- gauge_study %>%
  group_by(PROBE, WAFER, RUN) %>%
  filter(PROBE == 2362) %>%
  summarise(df = n()-1, probe_mean = mean(AVERAGE), probe_stdev = sd(AVERAGE), probe_stdev_sq = probe_s
  group_by(RUN) %>%
  summarise(s2_run = sqrt(mean(probe_stdev_sq)))
```

```
s2_2362
```

```
## # A tibble: 2 x 2
##   RUN s2_run
##   <int> <dbl>
## 1     1 0.0333
## 2     2 0.0388
```

Over both runs

```
s2_2352_all <- s2_2362 %>%
  mutate(s2_run_sq = s2_run^2) %$%
```

```

mean(s2_run_sq) %>%
sqrt()

s2_2352_all

## [1] 0.03616824

sd_2362_wafer <- gauge_study %>%
  group_by(PROBE, WAFER, RUN) %>%
  filter(PROBE == 2362) %>%
  summarise(probe_mean = mean(AVERAGE)) %>%
  mutate(
    run_number = case_when(
      RUN == 1 ~ "Run1",
      RUN == 2 ~ "Run2"
    )
  ) %>%
  dplyr::select(PROBE, WAFER, probe_mean, run_number) %>%
  group_by(WAFER) %>%
  summarise(sd_wafer = sd(probe_mean))

sd_2362_wafer

## # A tibble: 5 x 2
##   WAFER sd_wafer
##   <dbl>   <dbl>
## 1 138.  0.0222
## 2 139.  0.00271
## 3 140.  0.0288
## 4 141.  0.0133
## 5 142.  0.0205

s3_2362 <- sd_2362_wafer %>%
  mutate(sd_wafer_sq = sd_wafer^2) %$%
  mean(sd_wafer_sq) %>%
  sqrt()

s3_2362

## [1] 0.01964524

```





## Chapter 3

# Production Process Characterization

### 3.1 Packages used in this chapter

### 3.2 Case Studies

#### 3.2.1 Furnace Case Study

##### 3.2.1.1 Background and Data

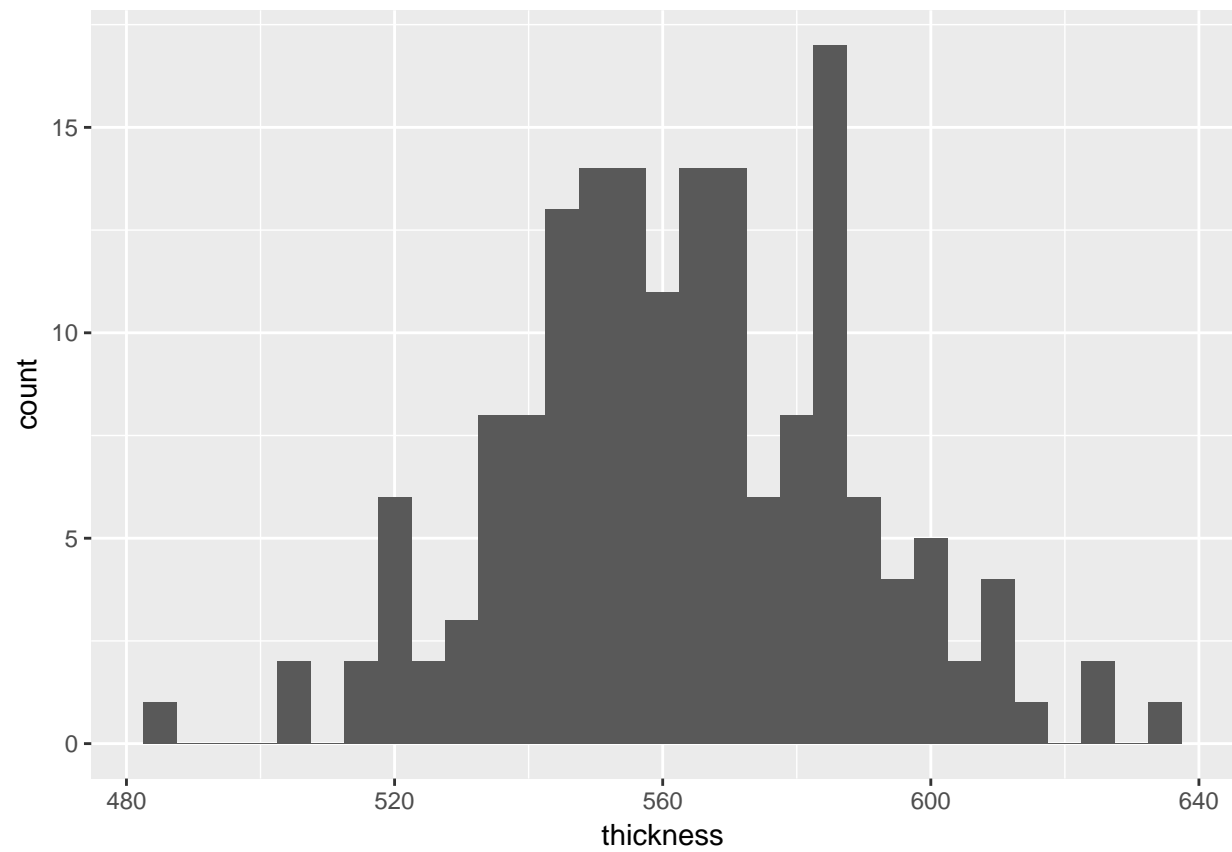
**Introduction** In a semiconductor manufacturing process flow, we have a step whereby we grow an oxide film on the silicon wafer using a furnace. In this step, a cassette of wafers is placed in a quartz “boat” and the boats are placed in the furnace. The furnace can hold four boats. A gas flow is created in the furnace and it is brought up to temperature and held there for a specified period of time (which corresponds to the desired oxide thickness). This study was conducted to determine if the process was stable and to characterize sources of variation so that a process control strategy could be developed.

The goal of this study is to determine if this process is capable of consistently growing oxide films with a thickness of 560 Angstroms  $\pm$  100 Angstroms. An additional goal is to determine important sources of variation for use in the development of a process control strategy.

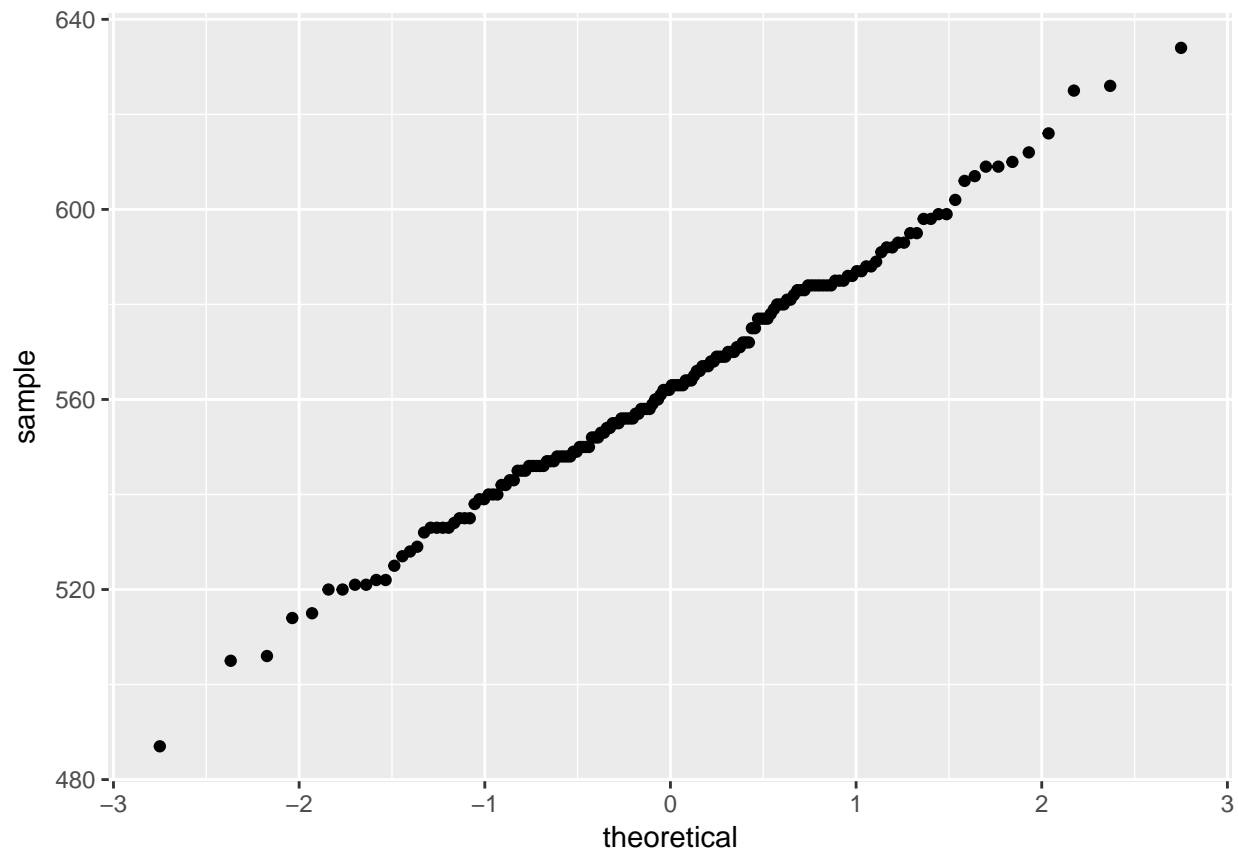
```
## Parsed with column specification:
## cols(
##   X1 = col_integer(),
##   X2 = col_integer(),
##   X3 = col_integer(),
##   X4 = col_integer()
## )
```

##### 3.2.1.2 Histogram and normal probability plots of all data

```
ggplot(data = furnace, mapping = aes(x = thickness)) +
  geom_histogram(binwidth = 5)
```



```
ggplot(data = furnace) +  
  geom_qq(aes(sample = thickness))
```



### 3.2.1.3 Summary statistics and standard deviation of film thickness

```
summary(furnace$thickness)
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  487.0   546.8   562.5   563.0   582.2   634.0
```

```
sd(furnace$thickness)
```

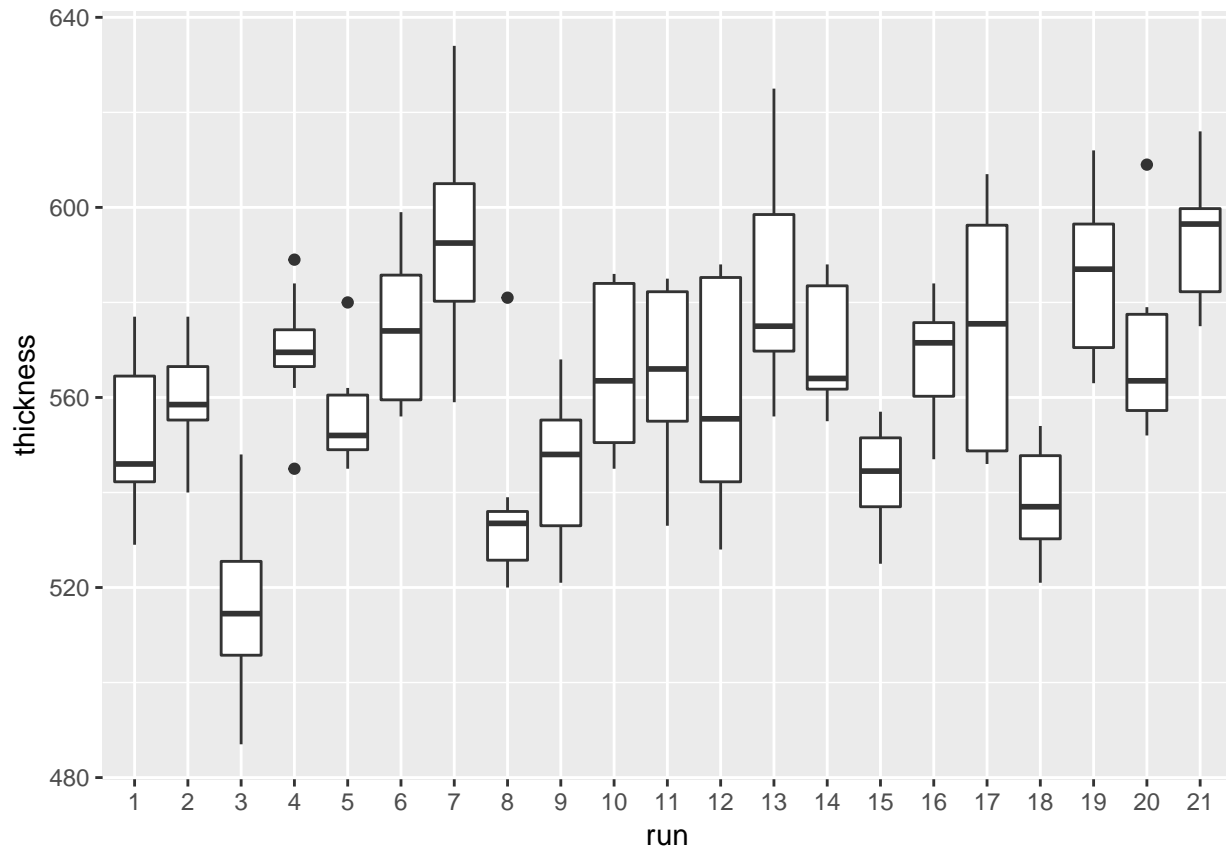
```
## [1] 25.38468
```

The NIST/SEMATECH e-Handbook ask for a capability analysis; however, this is covered in Chapter 6

### 3.2.1.4 Sources of variation

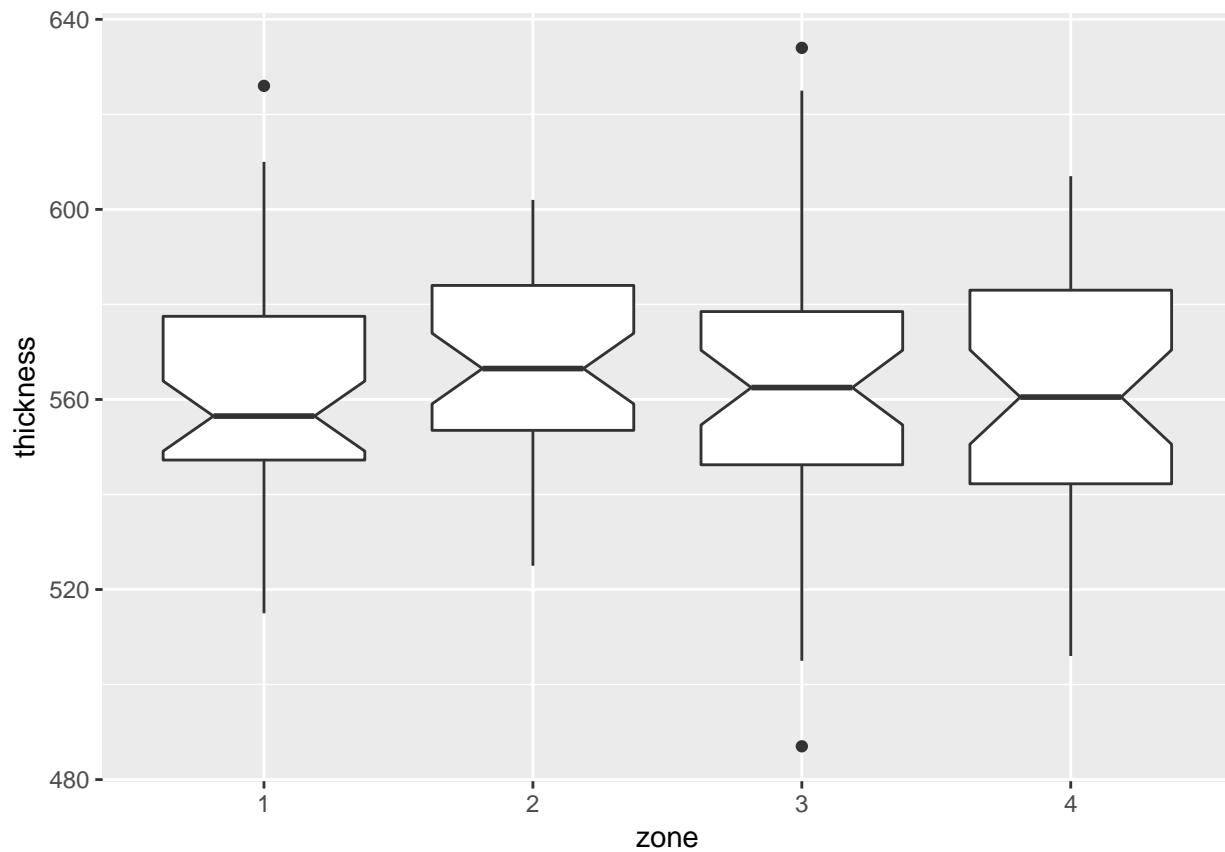
#### 3.2.1.4.1 Boxplot by run

```
ggplot(data = furnace, mapping = aes(x = run, y = thickness)) +
  geom_boxplot()
```



#### 3.2.1.4.2 Boxplot by zone

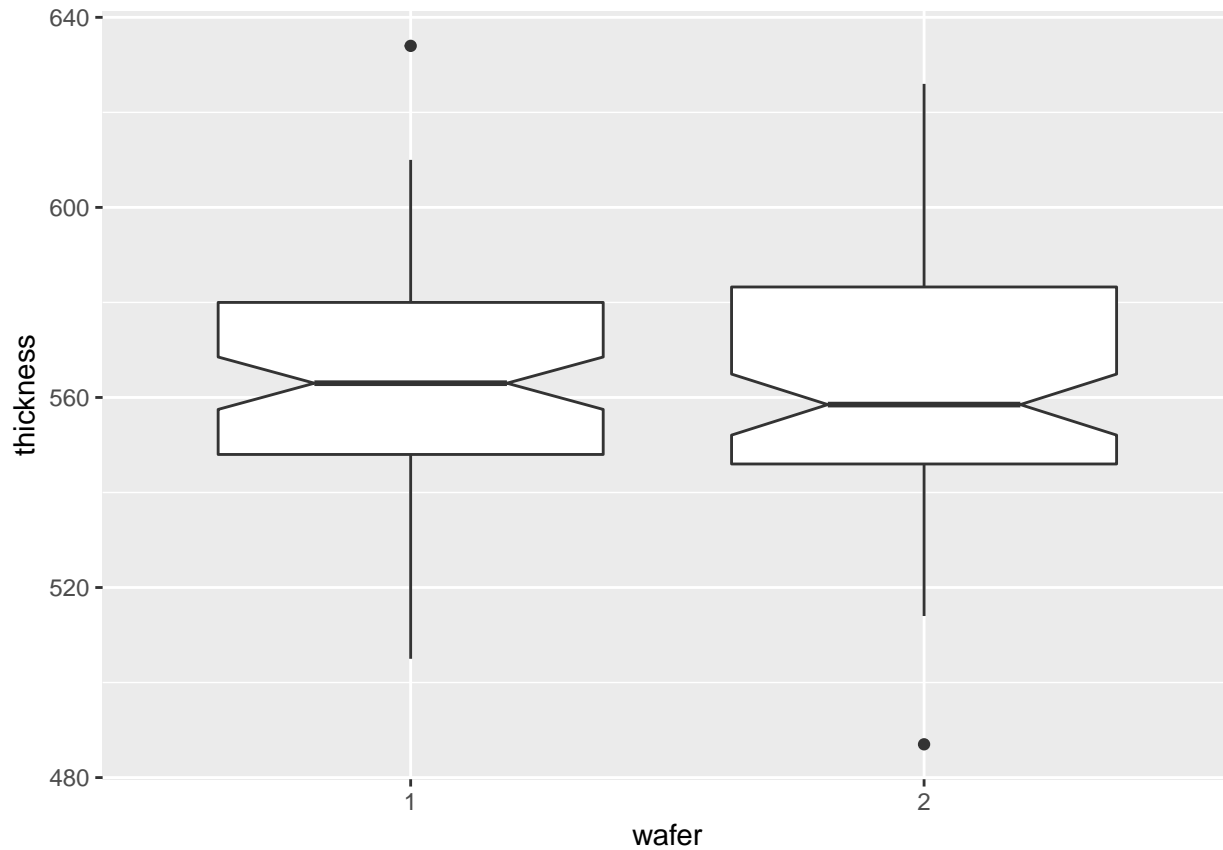
```
ggplot(data = furnace, mapping = aes(x = zone, y = thickness)) +  
  geom_boxplot(notch = TRUE)
```



**Notch** if FALSE (default) make a standard box plot. If TRUE, make a notched box plot. Notches are used to compare groups; if the notches of two boxes do not overlap, this suggests that the medians are significantly different.

#### 3.2.1.4.3 Boxplots by wafer

```
ggplot(data = furnace, mapping = aes(x = wafer, y = thickness)) +  
  geom_boxplot(notch = TRUE)
```



#### 3.2.1.4.4 One-way ANOVA to confirm thickness is different by run

```
aov.thickness <- aov(thickness ~ run, data = furnace)
summary(aov.thickness)
```

```
##              Df Sum Sq Mean Sq F value Pr(>F)
## run           20  61442   3072.1    9.781 <2e-16 ***
## Residuals    147   46170     314.1
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

#### 3.2.1.4.5 One-way ANOVA to confirm thickness is not different by zone

```
aov.zone <- aov(thickness ~ zone, data = furnace)
summary(aov.zone)
```

```
##              Df Sum Sq Mean Sq F value Pr(>F)
## zone           3     913     304.2    0.468  0.705
## Residuals    164 106699     650.6
```

#### 3.2.1.4.6 Nested ANOVA

```
aov.thickness.nested <- aov(thickness ~ run + run:zone, data = furnace)
summary(aov.thickness.nested)
```

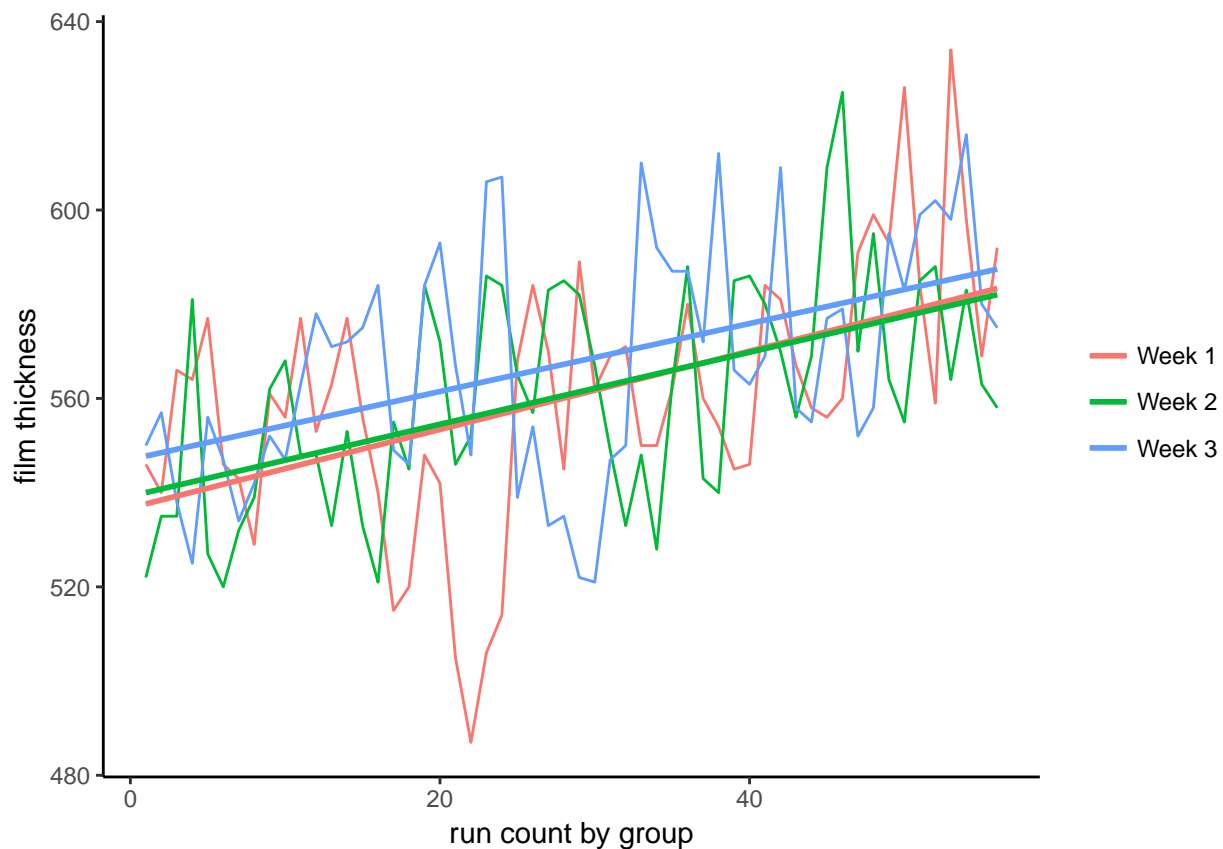
```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## run           20  61442   3072.1   25.412 < 2e-16 ***
```

```
## run:zone      63  36014   571.7   4.729 3.85e-11 ***
## Residuals    84  10155   120.9
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

### 3.2.1.4.7 Observed trend by week

```
furnace_group <- furnace %>%
  mutate(run = as.integer(run)) %>%
  mutate(grouping = case_when(run <= 7 ~ "Week 1",
                              run > 7 & run <= 14 ~ "Week 2",
                              run > 14 ~ "Week 3")) %>%
  mutate(counting = 1:n()) %>%
  # mutate(counting = as.double(counting)) %>%
  mutate(count_by_group = case_when(counting <= 56 ~ counting,
                                     counting > 56 & counting <= 112 ~ counting - 56L,
                                     counting > 112 ~ counting - 112L))

ggplot(furnace_group) +
  geom_line(aes(x = count_by_group, y = thickness, group = grouping, colour = grouping)) +
  geom_smooth(aes(x = count_by_group, y = thickness, group = grouping, colour = grouping),
             method = "lm", se = FALSE) +
  theme_classic() +
  theme(legend.title=element_blank()) +
  labs(x = "run count by group", y = "film thickness")
```



### 3.2.2 Machine Case Study

#### 3.2.2.1 Background and Data

**Background and Data Introduction** A machine shop has three automatic screw machines that produce various parts. The shop has enough capital to replace one of the machines. The quality control department has been asked to conduct a study and make a recommendation as to which machine should be replaced. It was decided to monitor one of the most commonly produced parts (an 1/8th inch diameter pin) on each of the machines and see which machine is the least stable.

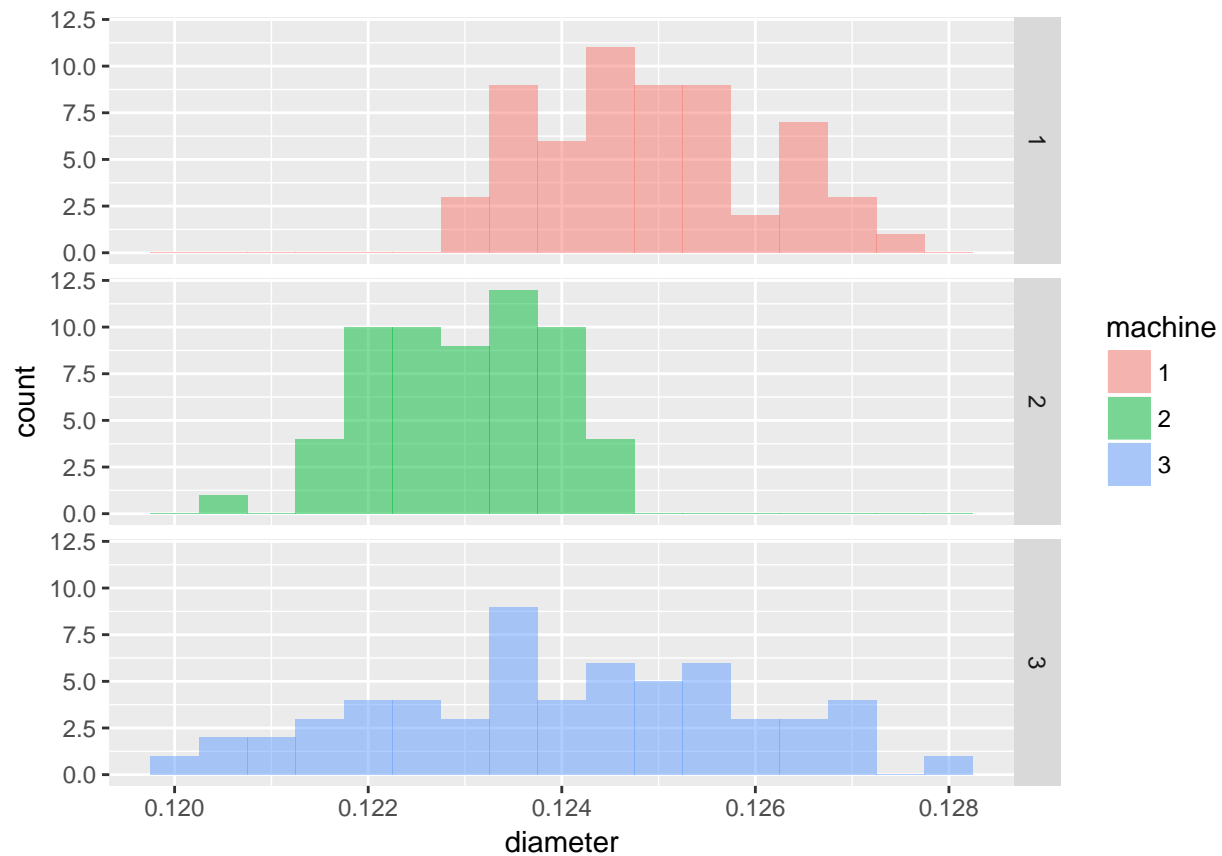
**Goal** The goal of this study is to determine which machine is least stable in manufacturing a steel pin with a diameter of .125 +/- .003 inches. Stability will be measured in terms of a constant variance about a constant mean. If all machines are stable, the decision will be based on process variability and throughput. Namely, the machine with the highest variability and lowest throughput will be selected for replacement.

```
## Parsed with column specification:
## cols(
##   X1 = col_integer(),
##   X2 = col_integer(),
##   X3 = col_integer(),
##   X4 = col_integer(),
##   X5 = col_double()
## )
```

#### 3.2.2.2 Histogram and normal probability plots of all data

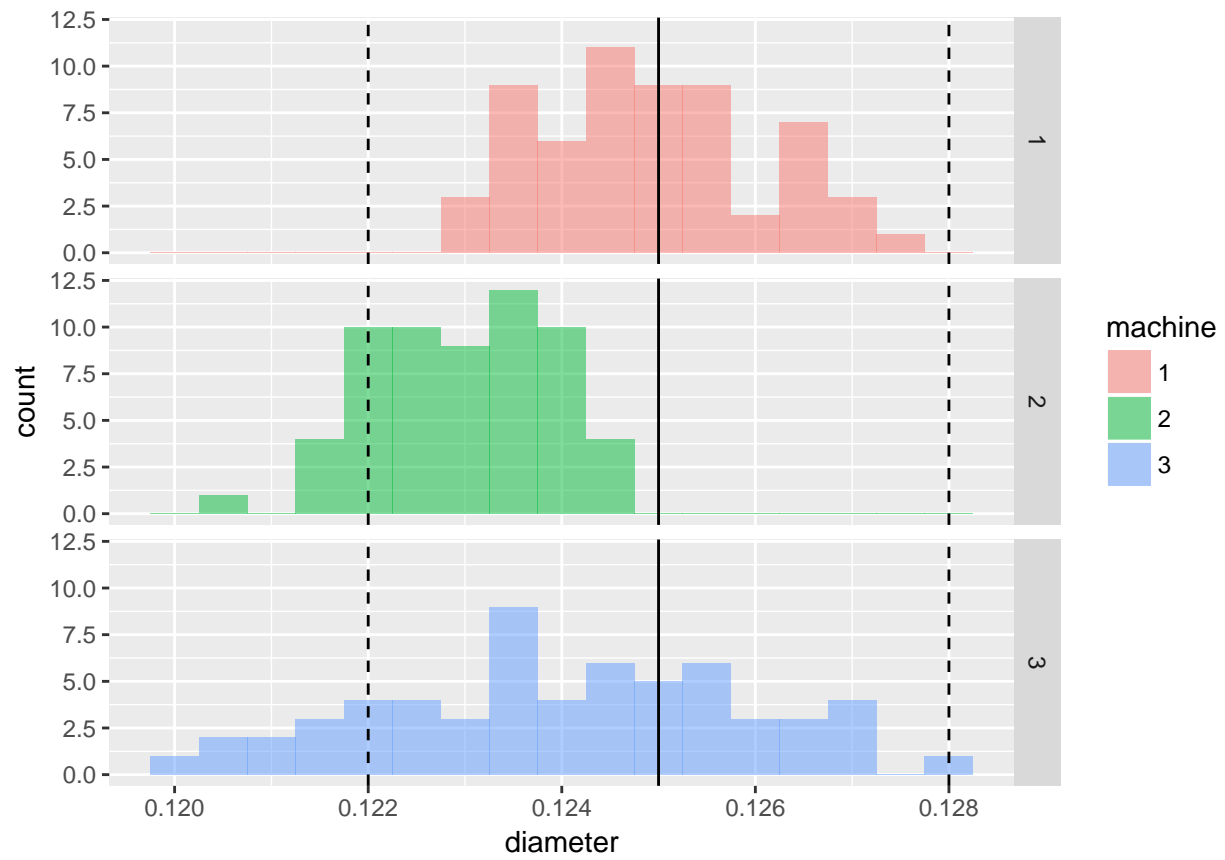
```
ggplot(machine, mapping = aes(x = diameter, fill = machine)) +
  geom_histogram(binwidth = 0.0005, alpha = 0.5) +
  facet_grid(machine ~ .)
```



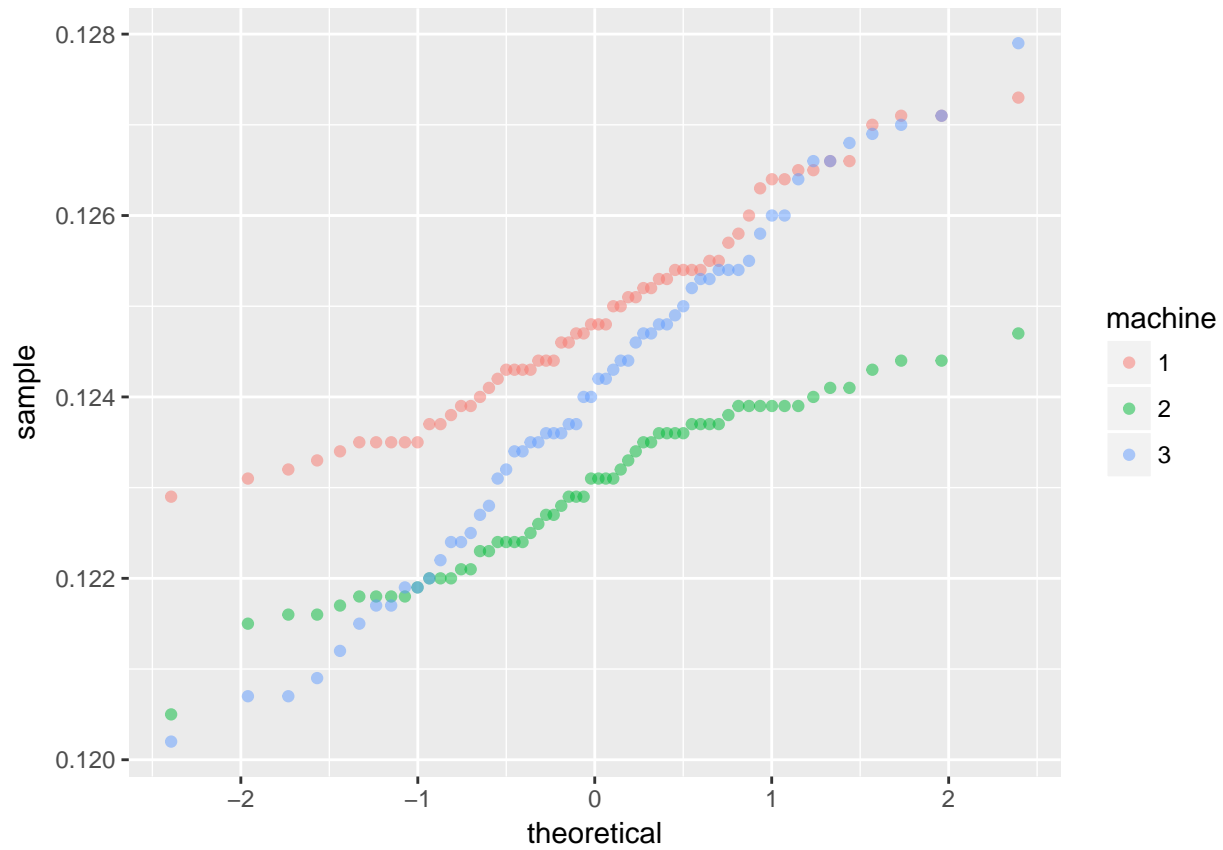


Since we are given the target diameter and tolerance, we can include these on the plot.

```
ggplot(machine, mapping = aes(x = diameter, fill = machine)) +
  geom_histogram(binwidth = 0.0005, alpha = 0.5) +
  geom_vline(aes(xintercept = 0.125)) +
  geom_vline(aes(xintercept = 0.128), linetype = 2) +
  geom_vline(aes(xintercept = 0.122), linetype = 2) +
  facet_grid(machine ~ .)
```



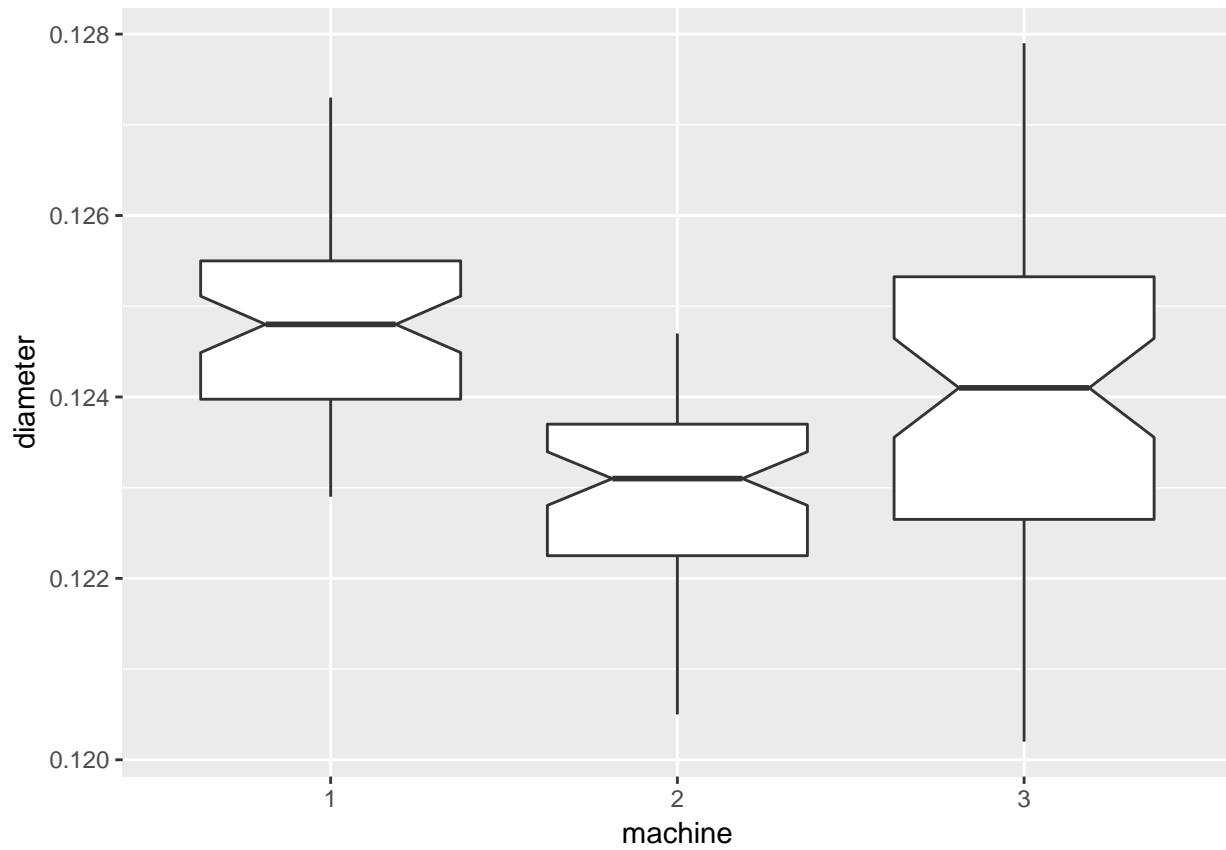
```
ggplot(machine, mapping = aes(colour = machine)) +  
  geom_qq(aes(sample = diameter), alpha = 0.5)
```



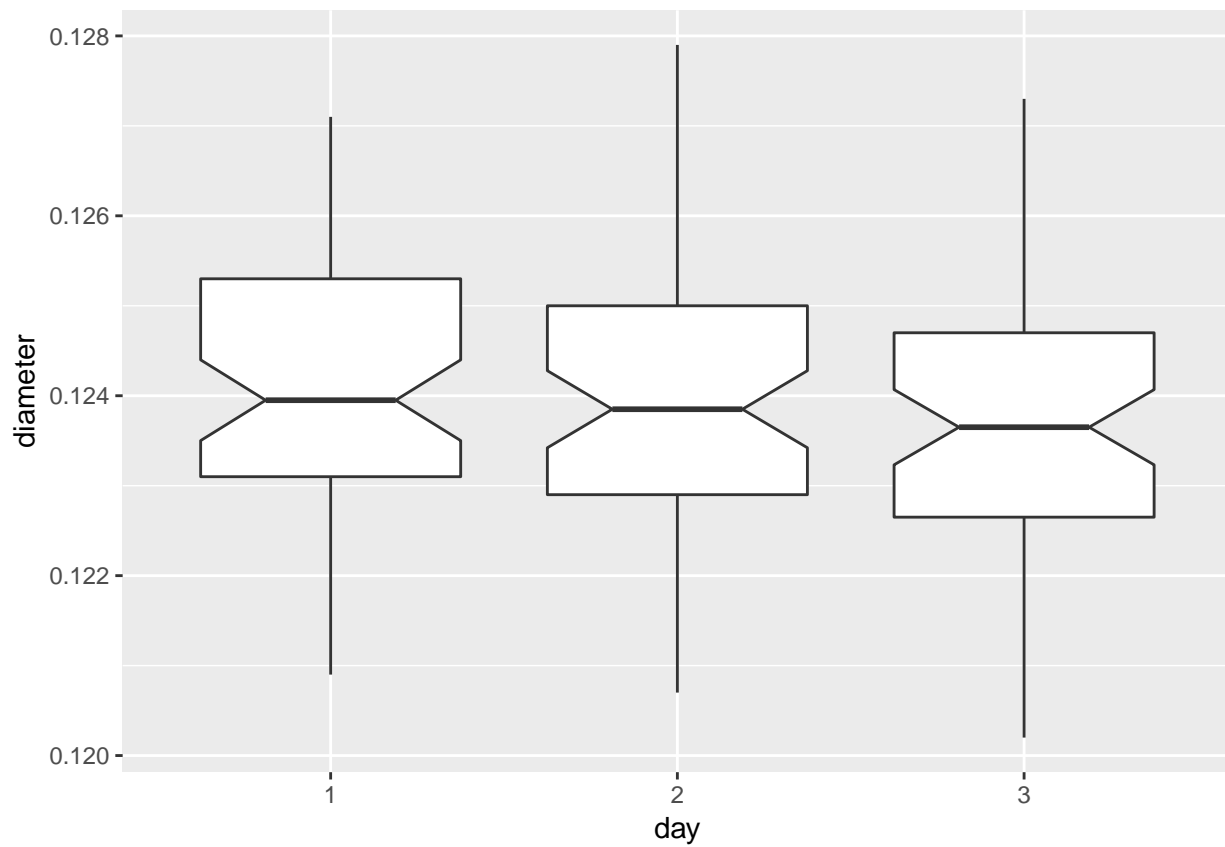
### 3.2.2.3 Sources of variation

#### 3.2.2.3.1 Boxplots by factors

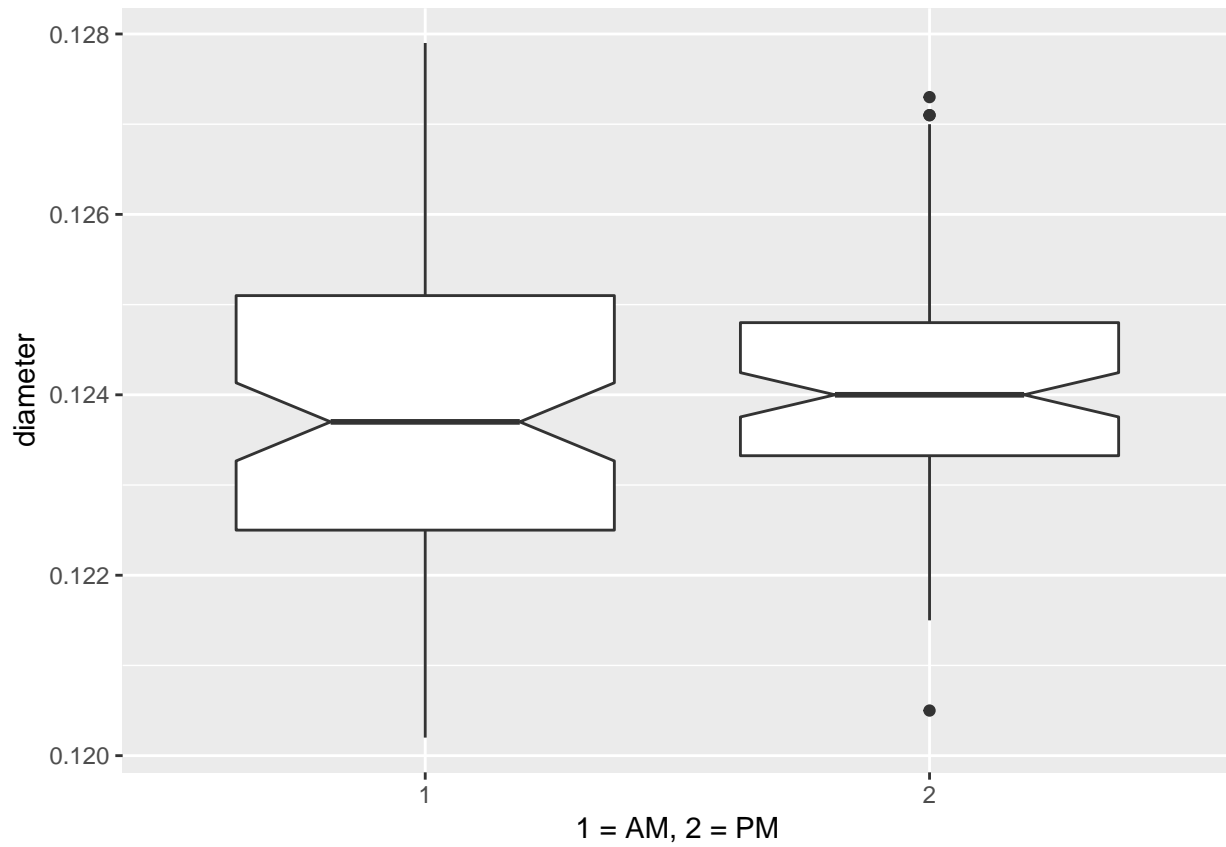
```
ggplot(data = machine, mapping = aes(x = machine, y = diameter)) +  
  geom_boxplot(notch = TRUE)
```



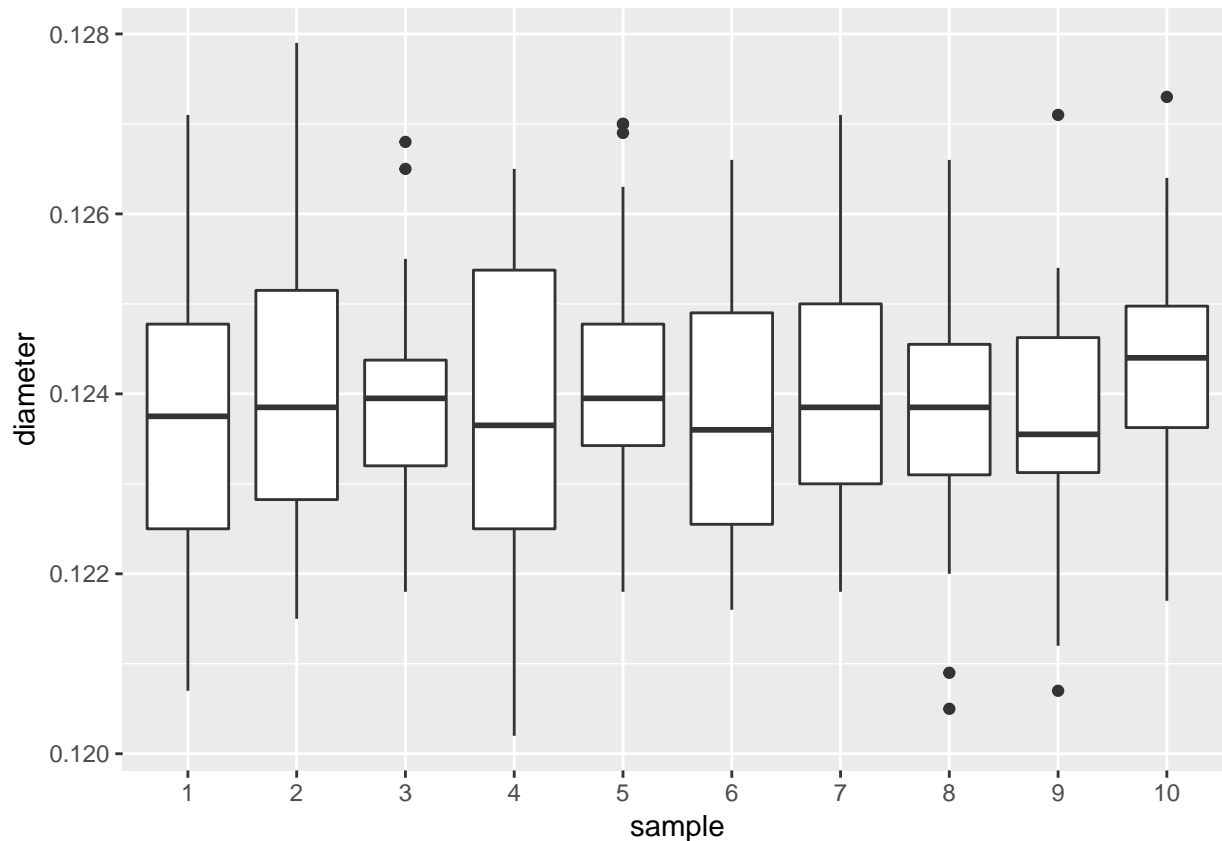
```
ggplot(data = machine, mapping = aes(x = day, y = diameter)) +  
  geom_boxplot(notch = TRUE)
```



```
ggplot(data = machine, mapping = aes(x = time, y = diameter)) +  
  geom_boxplot(notch = TRUE) +  
  labs(x = "1 = AM, 2 = PM")
```



```
ggplot(data = machine, mapping = aes(x = sample, y = diameter)) +  
  geom_boxplot(notch = FALSE)
```



### 3.2.2.3.2 ANOVA to confirm diameter by machine is different

```
aov.diameter <- aov(diameter ~ machine + day + time + sample, data = machine)
summary(aov.diameter)
```

```
##           Df    Sum Sq  Mean Sq F value    Pr(>F)
## machine      2 1.107e-04 5.538e-05 29.316 1.28e-11 ***
## day          2 3.730e-06 1.870e-06  0.988  0.374
## time         1 2.360e-06 2.360e-06  1.248  0.266
## sample       9 8.850e-06 9.800e-07  0.521  0.858
## Residuals   165 3.117e-04 1.890e-06
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
aov.diameter.machine <- aov(diameter ~ machine, data = machine)
summary(aov.diameter.machine)
```

```
##           Df    Sum Sq  Mean Sq F value    Pr(>F)
## machine      2 0.0001108 5.538e-05 30.01 5.99e-12 ***
## Residuals   177 0.0003266 1.850e-06
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```





## Chapter 4

# Modeling

### 4.1 Packages used in this chapter

```
library(tidyverse)
library(ggplot2)
library(broom)
```

### 4.2 Introduction

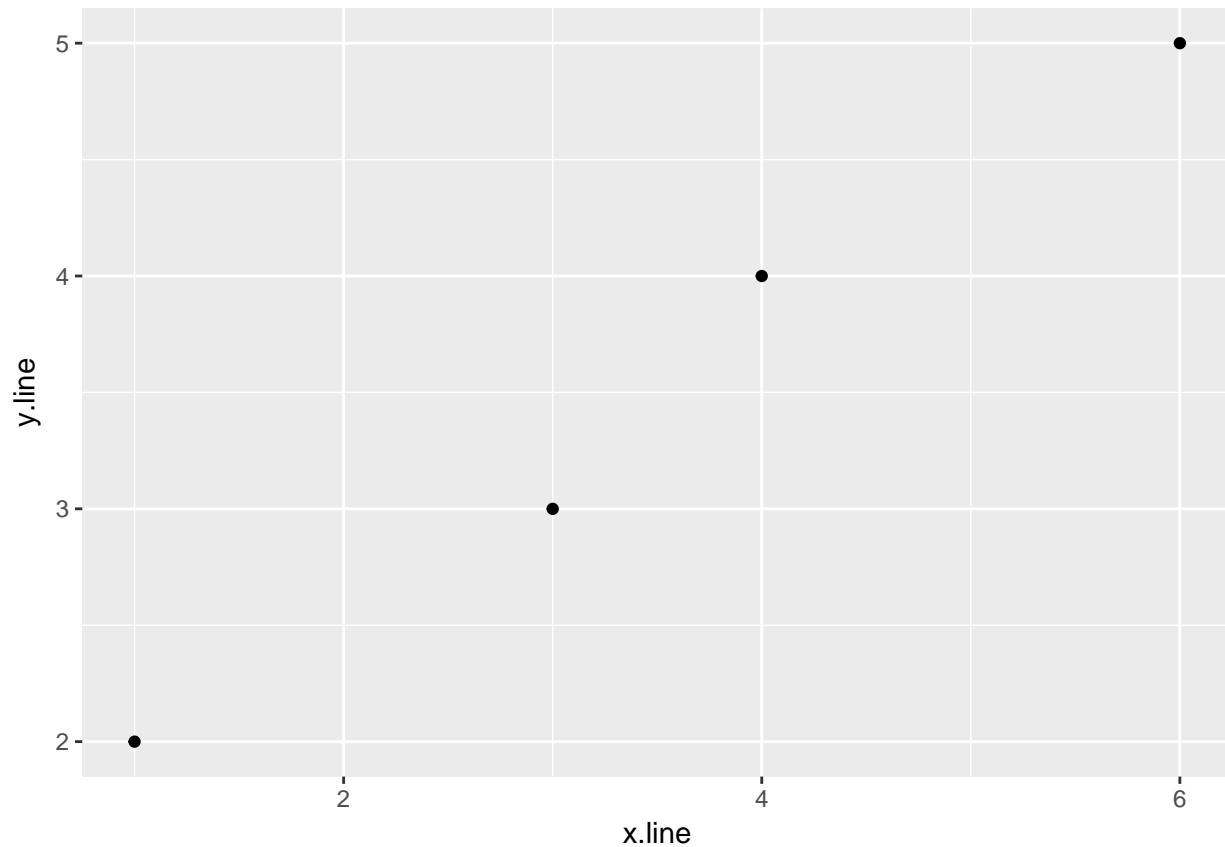
#### 4.2.1 A simple linear regression model

```
simple_line <- tribble(
  ~x.line, ~y.line,
  1., 2.,
  3., 3.,
  4., 4.,
  6., 5.
)
simple_line
```

```
## # A tibble: 4 x 2
##   x.line y.line
##   <dbl> <dbl>
## 1     1.     2.
## 2     3.     3.
## 3     4.     4.
## 4     6.     5.
```

##### 4.2.1.1 Plot of the data

```
ggplot(simple_line, aes(x.line, y.line)) +
  geom_point()
```



#### 4.2.1.2 Linear regression

Below, the data is fit to the line

$$y = mx + b$$

the intercept is assumed unless explicitly removed using either  $y \sim x - 1$  or  $y \sim 0 + x$ .

```
m_sl <- lm(y.line ~ x.line,
           data = simple_line)
m_sl
```

```
##
## Call:
## lm(formula = y.line ~ x.line, data = simple_line)
##
## Coefficients:
## (Intercept)      x.line
##      1.3462      0.6154
```

```
summary(m_sl)
```

```
##
## Call:
## lm(formula = y.line ~ x.line, data = simple_line)
##
## Residuals:
```

```
##           1           2           3           4
## 0.03846 -0.19231  0.19231 -0.03846
##
## Coefficients:
##           Estimate Std. Error t value Pr(>|t|)
## (Intercept)  1.34615    0.21414   6.286  0.02438 *
## x.line       0.61538    0.05439  11.314  0.00772 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.1961 on 2 degrees of freedom
## Multiple R-squared:  0.9846, Adjusted R-squared:  0.9769
## F-statistic: 128 on 1 and 2 DF, p-value: 0.007722
```

```
tidy(m_sl)
```

```
##           term estimate std.error statistic    p.value
## 1 (Intercept) 1.3461538 0.21414478   6.286186 0.024384322
## 2      x.line 0.6153846 0.05439283  11.313708 0.007722123
```

```
sl_slope <- tidy(m_sl) %>%
  filter(term == "x.line") %>%
  dplyr::select(estimate)

sl_intercept <- tidy(m_sl) %>%
  filter(term == "(Intercept)") %>%
  dplyr::select(estimate)

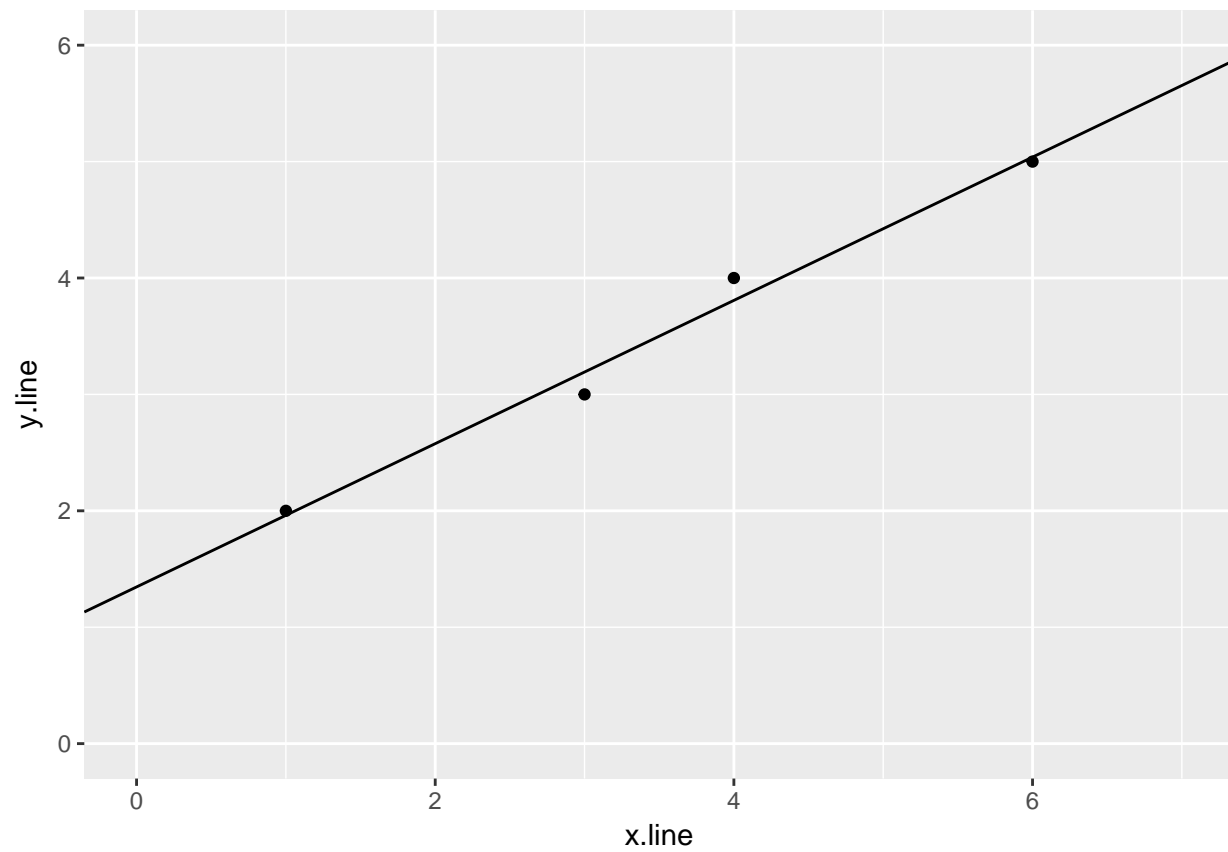
sl_slope
```

```
##      estimate
## 1 0.6153846
sl_intercept
```

```
##      estimate
## 1 1.346154
```

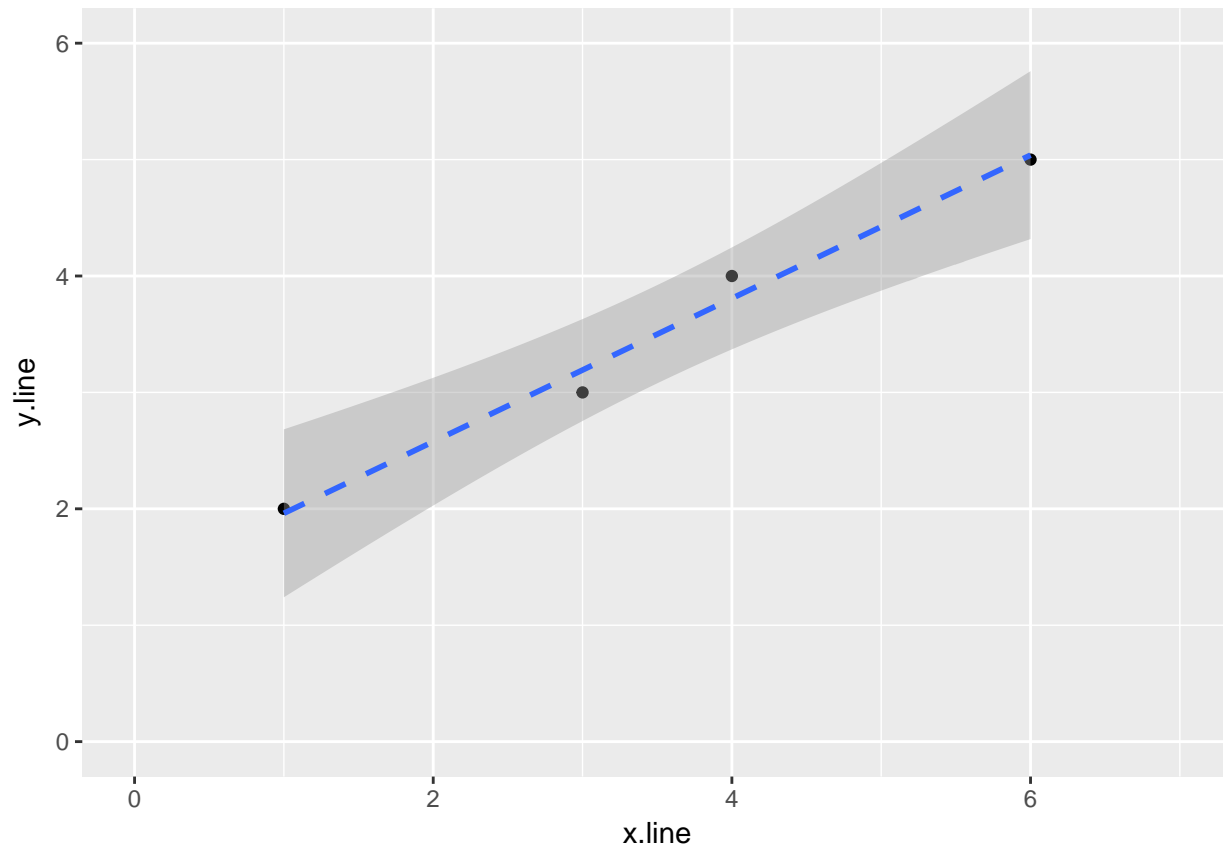
#### 4.2.1.3 Plot of the data and linear regression

```
ggplot(simple_line, aes(x.line, y.line)) +
  geom_point() +
  geom_abline(slope = sl_slope$estimate, intercept = sl_intercept$estimate) +
  ylim(0,6) +
  xlim(0,7)
```



If we don't need the coefficients, we can plot the data and linear regression using ggplot2

```
ggplot(simple_line, aes(x.line, y.line)) +  
  geom_point() +  
  stat_smooth(method = lm, linetype = "dashed") +  
  ylim(0,6) +  
  xlim(0,7)
```



#### 4.2.1.4 Finally, let's add prediction intervals to the graph

```
temp_var <- m_sl %>%
  predict(interval="predict") %>%
  as_tibble()
```

```
## Warning in predict.lm(., interval = "predict"): predictions on current data refer to _future_ responses
```

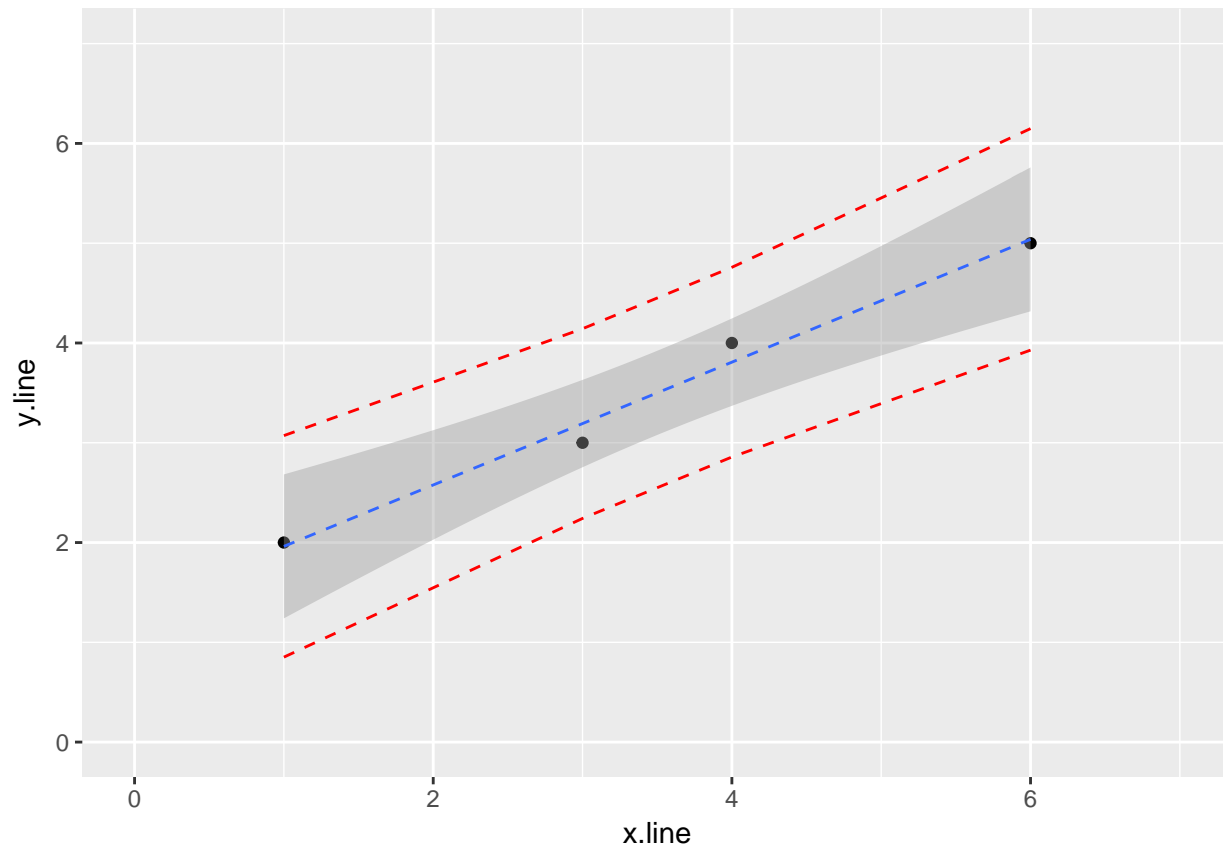
```
temp_var
```

```
## # A tibble: 4 x 3
##   fit lwr upr
##   <dbl> <dbl> <dbl>
## 1  1.96 0.851 3.07
## 2  3.19 2.24 4.14
## 3  3.81 2.86 4.76
## 4  5.04 3.93 6.15
```

```
simple_line_predict <- bind_cols(simple_line, temp_var)
simple_line_predict
```

```
## # A tibble: 4 x 5
##   x.line y.line fit lwr upr
##   <dbl> <dbl> <dbl> <dbl> <dbl>
## 1     1.     2.  1.96 0.851 3.07
## 2     3.     3.  3.19 2.24 4.14
## 3     4.     4.  3.81 2.86 4.76
```

```
## 4      6.      5.  5.04 3.93  6.15
ggplot(simple_line_predict, aes(x.line, y.line)) +
  geom_point() +
  stat_smooth(method = lm, linetype = "dashed", size = 0.5) +
  geom_line(aes(y=lwr), color = "red", linetype = "dashed") +
  geom_line(aes(y=upr), color = "red", linetype = "dashed") +
  ylim(0,7) +
  xlim(0,7)
```



## 4.2.2 Beyond the linear regression

### 4.2.2.1 A simple data set for non-linear regression modeling—exponential decay

Example is from Brown, LeMay.

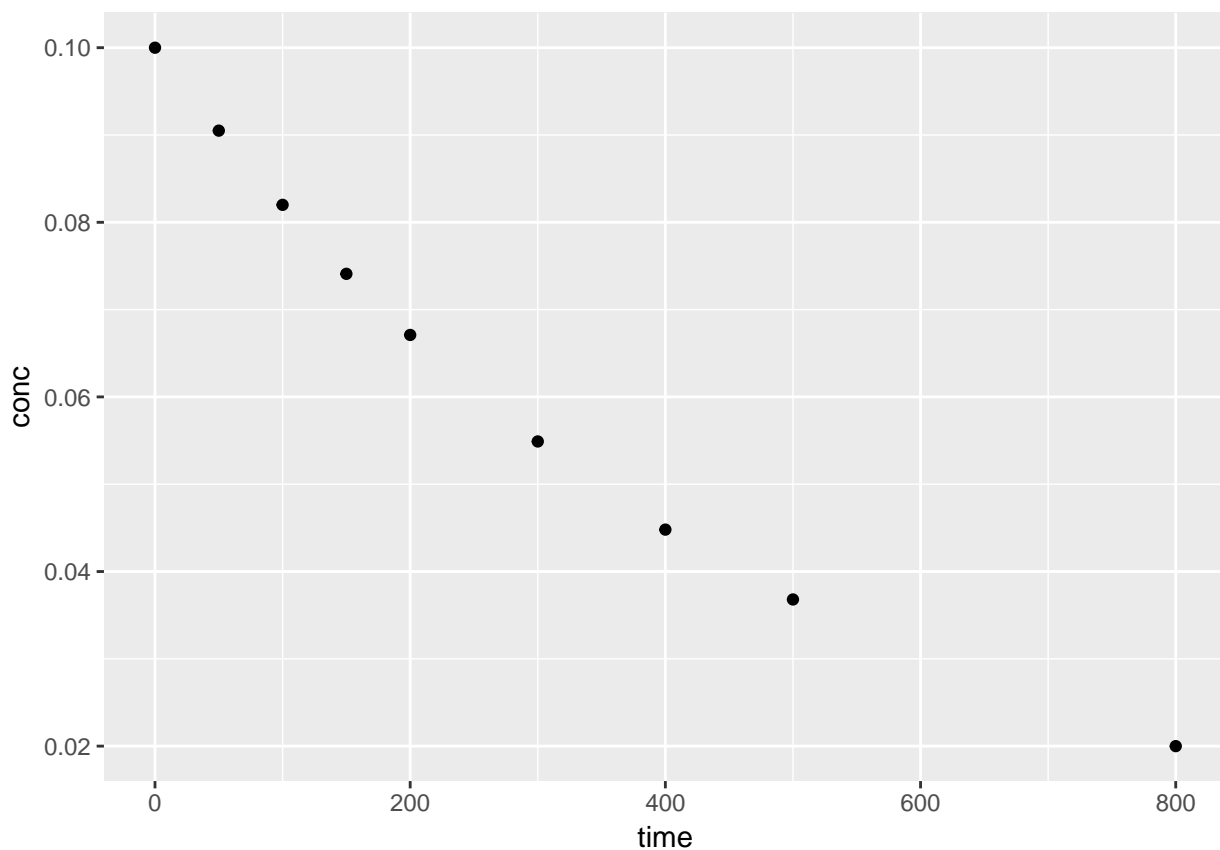
```
kinetics1 <- tribble(
  ~time, ~conc,
  0., 0.100,
  50., 0.0905,
  100., 0.0820,
  150., 0.0741,
  200., 0.0671,
  300., 0.0549,
  400., 0.0448,
  500., 0.0368,
  800., 0.0200
```

```
)  
kinetics1  
  
## # A tibble: 9 x 2  
##   time  conc  
##   <dbl> <dbl>  
## 1    0. 0.100  
## 2   50. 0.0905  
## 3  100. 0.0820  
## 4  150. 0.0741  
## 5  200. 0.0671  
## 6  300. 0.0549  
## 7  400. 0.0448  
## 8  500. 0.0368  
## 9  800. 0.0200
```

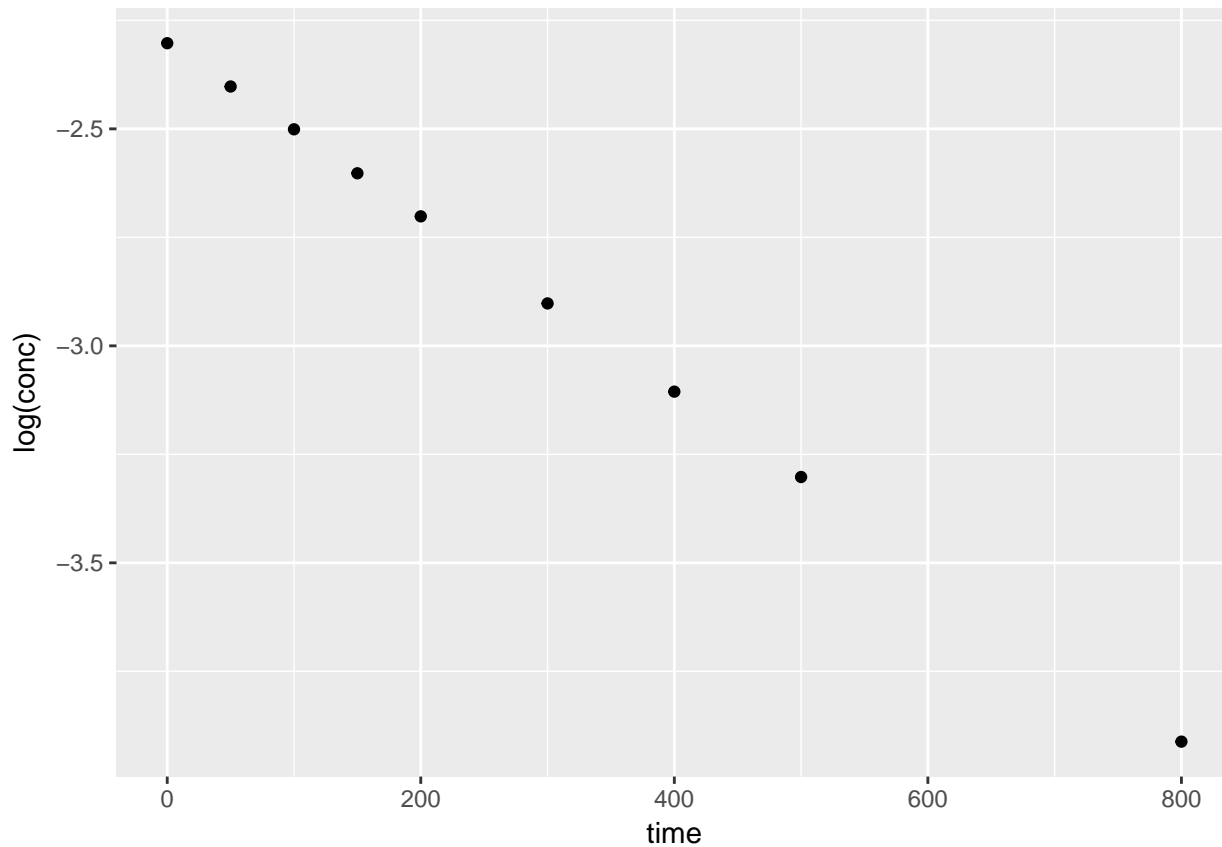
#### 4.2.2.2 Simple plots of the data

We can plot the original data set, conc vs. time to view the trend. A simple test to confirm the data follows a first-order decay, we can plot  $\log(\text{conc})$  vs. time.

```
ggplot(kinetics1, aes(time, conc)) +  
  geom_point()
```



```
ggplot(kinetics1, aes(time, log(conc))) +  
  geom_point()
```



#### 4.2.2.3 Using the nls function

```
k1 <- nls(conc ~ 0.1*exp(-a1*time),
          data = kinetics1, start = list(a1 = 0.002), trace = T)
```

```
## 7.545743e-08 : 0.002
## 7.088224e-08 : 0.0020017
## 7.088224e-08 : 0.002001699
```

```
summary(k1)
```

```
##
## Formula: conc ~ 0.1 * exp(-a1 * time)
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## a1 2.002e-03  2.367e-06   845.8   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.413e-05 on 8 degrees of freedom
##
## Number of iterations to convergence: 2
## Achieved convergence tolerance: 2.138e-07
```



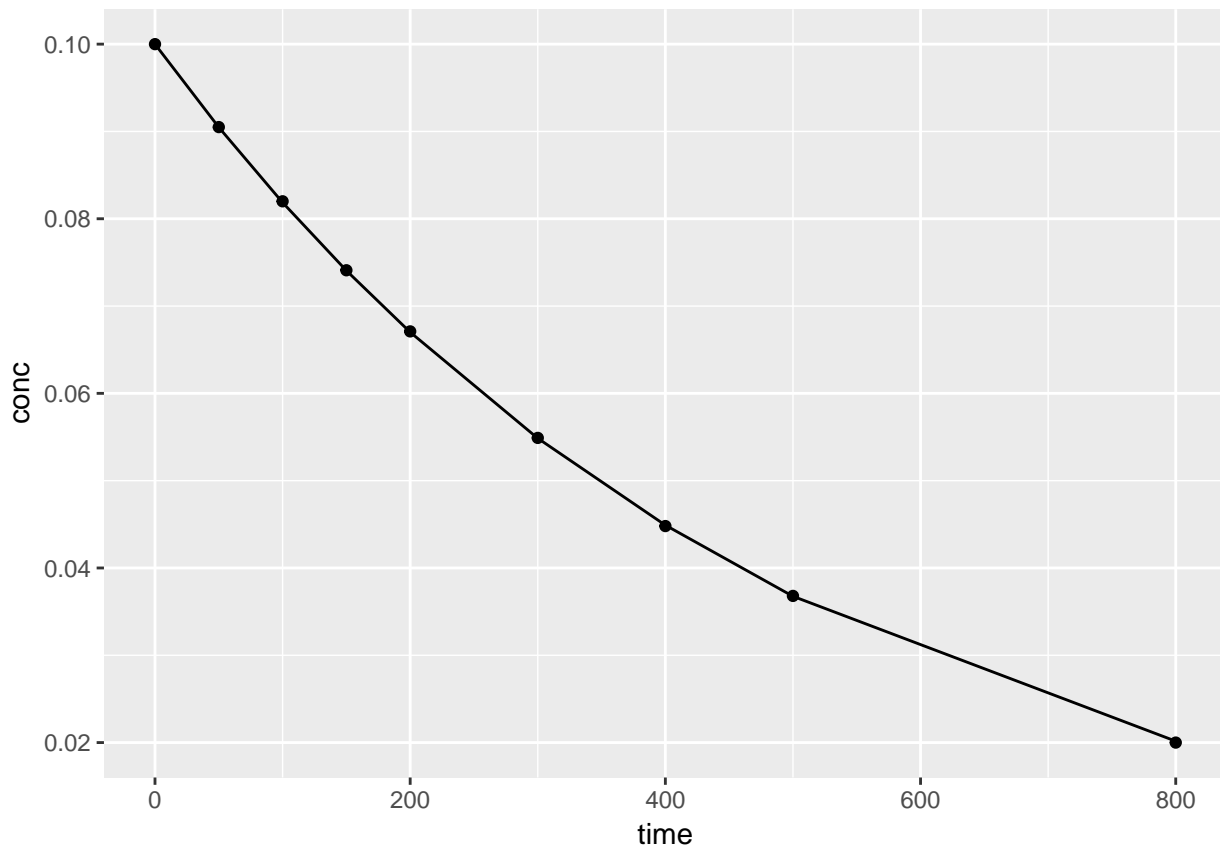
#### 4.2.2.4 Plotting the model results

Using the `augment()` function from the **broom** package, we can plot both the data and predicted values from the `nls()` model.

```
augment(k1)
```

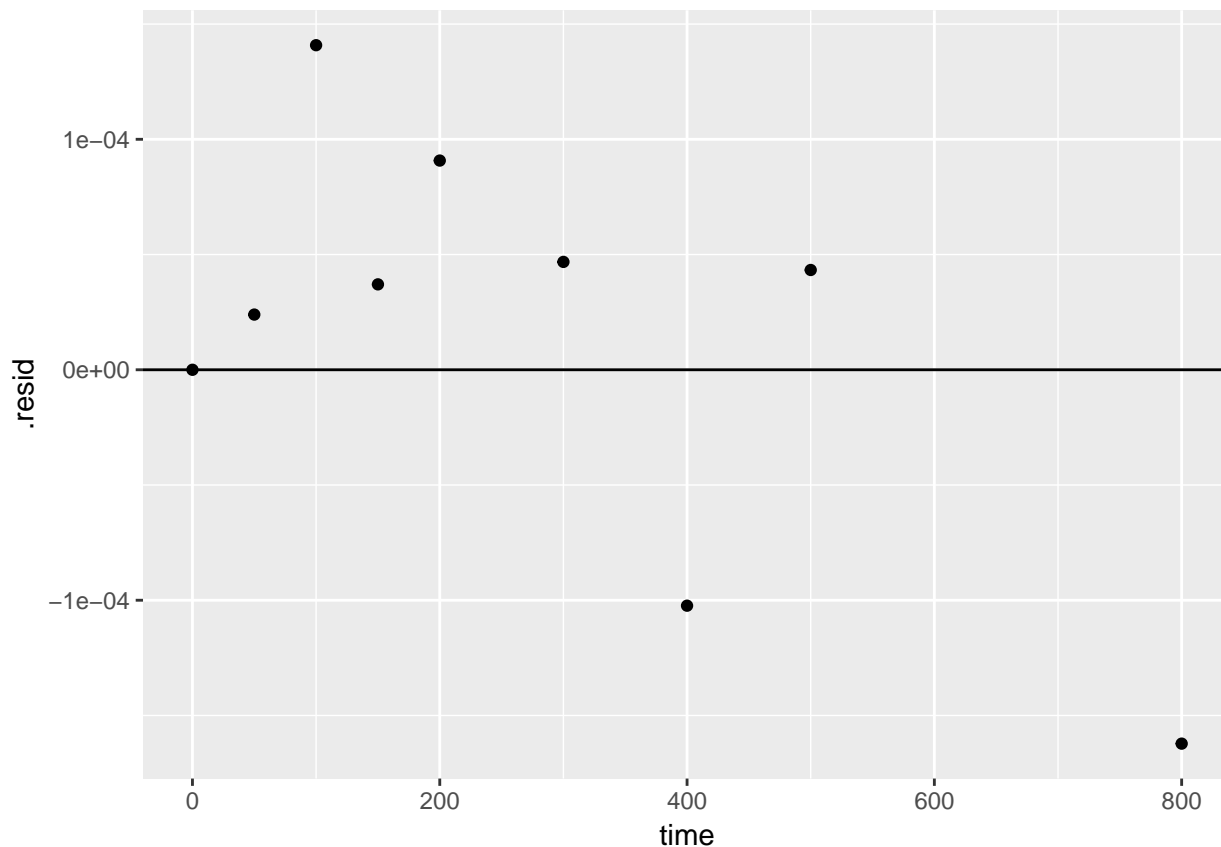
```
##   time  conc   .fitted   .resid
## 1    0 0.1000 0.10000000 0.000000e+00
## 2   50 0.0905 0.09047605 2.394510e-05
## 3  100 0.0820 0.08185917 1.408349e-04
## 4  150 0.0741 0.07406294 3.705685e-05
## 5  200 0.0671 0.06700923 9.077090e-05
## 6  300 0.0549 0.05485320 4.680452e-05
## 7  400 0.0448 0.04490237 -1.023678e-04
## 8  500 0.0368 0.03675670 4.329657e-05
## 9  800 0.0200 0.02016223 -1.622264e-04
```

```
ggplot()+
  geom_point(aes(time, conc), kinetics1) +
  geom_line(aes(time, .fitted), augment(k1))
```



We can also use the output of `augment()` to plot the residuals

```
ggplot()+
  geom_point(aes(time, .resid), augment(k1)) +
  geom_hline(yintercept = 0)
```



#### 4.2.2.4.1 create a function for the fit

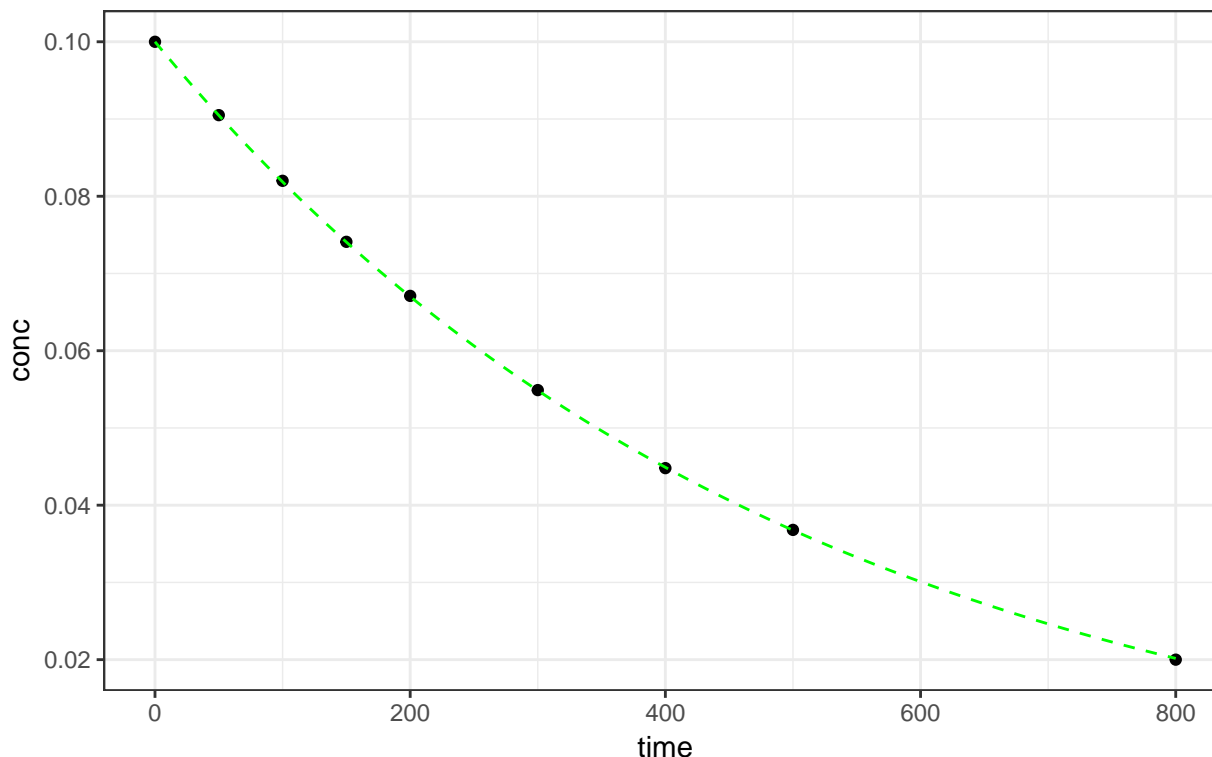
If we want to create a smooth curve of the fit, we need to create a function and use the calculated coefficients from the `nls()` model. We can then use the `stat_function()` geom to superimpose the function on the base plot.

```
conc.fit <- function(t) {
  0.1*exp(-t*summary(k1)$coefficients[1])
}

ggplot(kinetics1, mapping = aes(time, conc)) +
  geom_point() +
  stat_function(fun = conc.fit, linetype = "dashed", colour = "green") +
  ggtitle("A kinetics example from first-year chemistry", subtitle = "dashed green line: first-order, e")
  theme_bw()
```

### A kinetics example from first-year chemistry

dashed green line: first-order, exponential decay



## 4.3 Case Studies

### 4.3.1 Load cell output

Load cell calibration

The data collected in the calibration experiment consisted of a known load, applied to the load cell, and the corresponding deflection of the cell from its nominal position. Forty measurements were made over a range of loads from 150,000 to 3,000,000 units. The data were collected in two sets in order of increasing load. The systematic run order makes it difficult to determine whether or not there was any drift in the load cell or measuring equipment over time. Assuming there is no drift, however, the experiment should provide a good description of the relationship between the load applied to the cell and its response.

```
library(tidyverse)

load_cell <- read_table2(
  "NIST data/PONTIUS.dat", skip = 25, col_names = FALSE, col_types = "dd") %>%
  rename(Deflection = X1, Load = X2)
load_cell

## # A tibble: 40 x 2
##   Deflection    Load
##   <dbl>      <dbl>
## 1    0.110  150000.
## 2    0.220  300000.
```

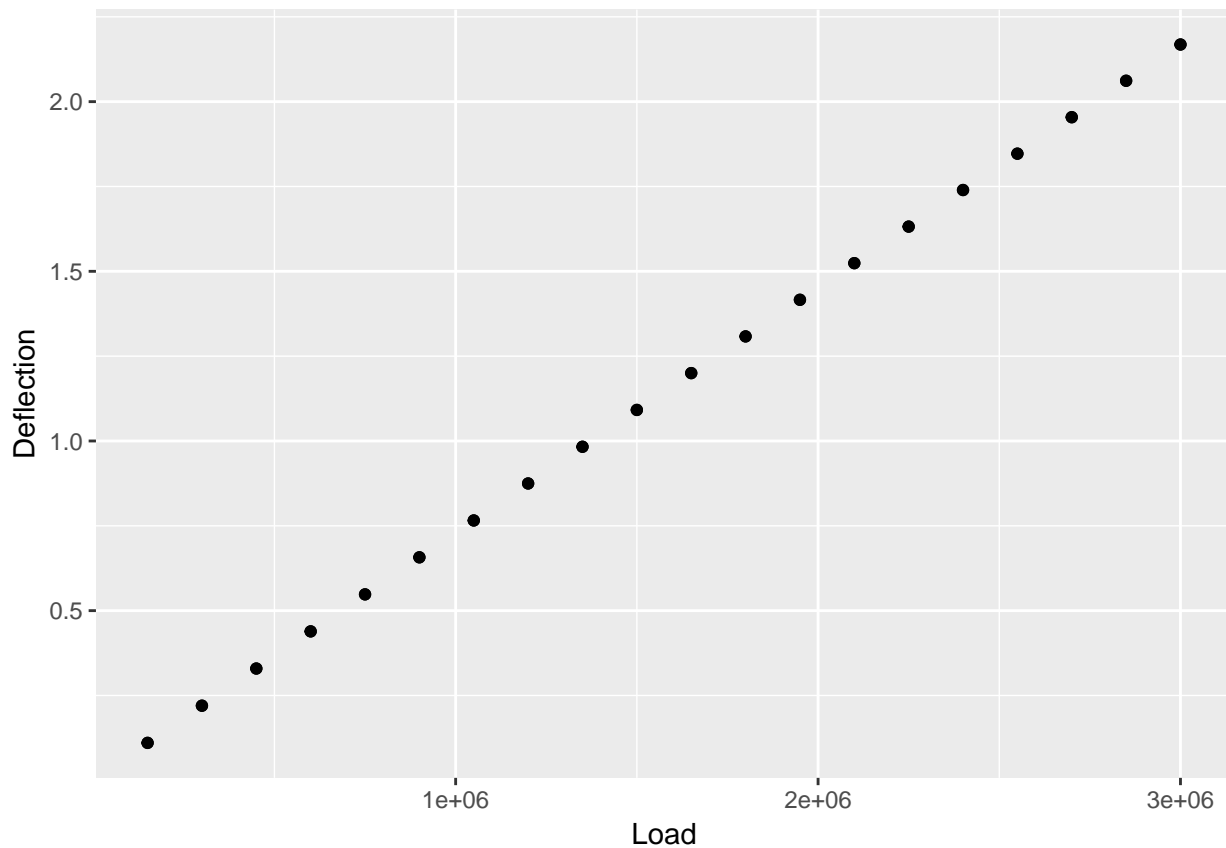
```
## 3      0.329 450000.
## 4      0.439 600000.
## 5      0.548 750000.
## 6      0.657 900000.
## 7      0.766 1050000.
## 8      0.875 1200000.
## 9      0.983 1350000.
## 10     1.09 1500000.
## # ... with 30 more rows
```

---

#### 4.3.1.1 Selection of Initial Model

First, let's view the data.

```
ggplot(load_cell) +
  geom_point(aes(Load, Deflection))
```



The data looks linear. We can use a simple linear model to view the data

$$y = mx + b$$

```
load_cell_model <- lm(Deflection ~ Load, load_cell)
summary(load_cell_model)
```

```
##
```

```
## Call:
## lm(formula = Deflection ~ Load, data = load_cell)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0042751 -0.0016308  0.0005818  0.0018932  0.0024211
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 6.150e-03  7.132e-04   8.623 1.77e-10 ***
## Load       7.221e-07  3.969e-10 1819.289 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.002171 on 38 degrees of freedom
## Multiple R-squared:  1, Adjusted R-squared:  1
## F-statistic: 3.31e+06 on 1 and 38 DF, p-value: < 2.2e-16
```

Wow! an R-squared value of 1! it must be perfect.

#### 4.3.1.1.1 A new package to work with summary information: broom()

**broom** package is part of the tidyverse and includes `glance()`, `tidy`, and `augment()`. These functions create tidy data frames based on the model.

```
load_cell_glance <- glance(load_cell_model)
load_cell_glance
```

```
##   r.squared adj.r.squared      sigma statistic      p.value df logLik
## 1 0.9999885    0.9999882 0.002171273   3309811 1.773069e-95  2 189.566
##      AIC      BIC    deviance df.residual
## 1 -373.132 -368.0654 0.0001791481         38
```

```
load_cell_tidy <- tidy(load_cell_model)
load_cell_tidy
```

```
##      term      estimate  std.error  statistic      p.value
## 1 (Intercept) 6.149684e-03 7.132052e-04   8.622602 1.772153e-10
## 2      Load 7.221026e-07 3.969148e-10 1819.288717 1.773069e-95
```

```
augment(load_cell_model)
```

```
##   Deflection  Load  .fitted  .se.fit  .resid  .hat
## 1    0.11019 150000 0.1144651 0.0006616404 -0.0042750714 0.09285714
## 2    0.21956 300000 0.2227805 0.0006115258 -0.0032204586 0.07932331
## 3    0.32949 450000 0.3310958 0.0005632485 -0.0016058459 0.06729323
## 4    0.43899 600000 0.4394112 0.0005173233 -0.0004212331 0.05676692
## 5    0.54803 750000 0.5477266 0.0004744336  0.0003033797 0.04774436
## 6    0.65694 900000 0.6560420 0.0004354772  0.0008979925 0.04022556
## 7    0.76562 1050000 0.7643574 0.0004016005  0.0012626053 0.03421053
## 8    0.87487 1200000 0.8726728 0.0003741856  0.0021972180 0.02969925
## 9    0.98292 1350000 0.9809882 0.0003547339  0.0019318308 0.02669173
## 10   1.09146 1500000 1.0893036 0.0003445966  0.0021564436 0.02518797
## 11   1.20001 1650000 1.1976189 0.0003445966  0.0023910564 0.02518797
## 12   1.30822 1800000 1.3059343 0.0003547339  0.0022856692 0.02669173
## 13   1.41599 1950000 1.4142497 0.0003741856  0.0017402820 0.02969925
```

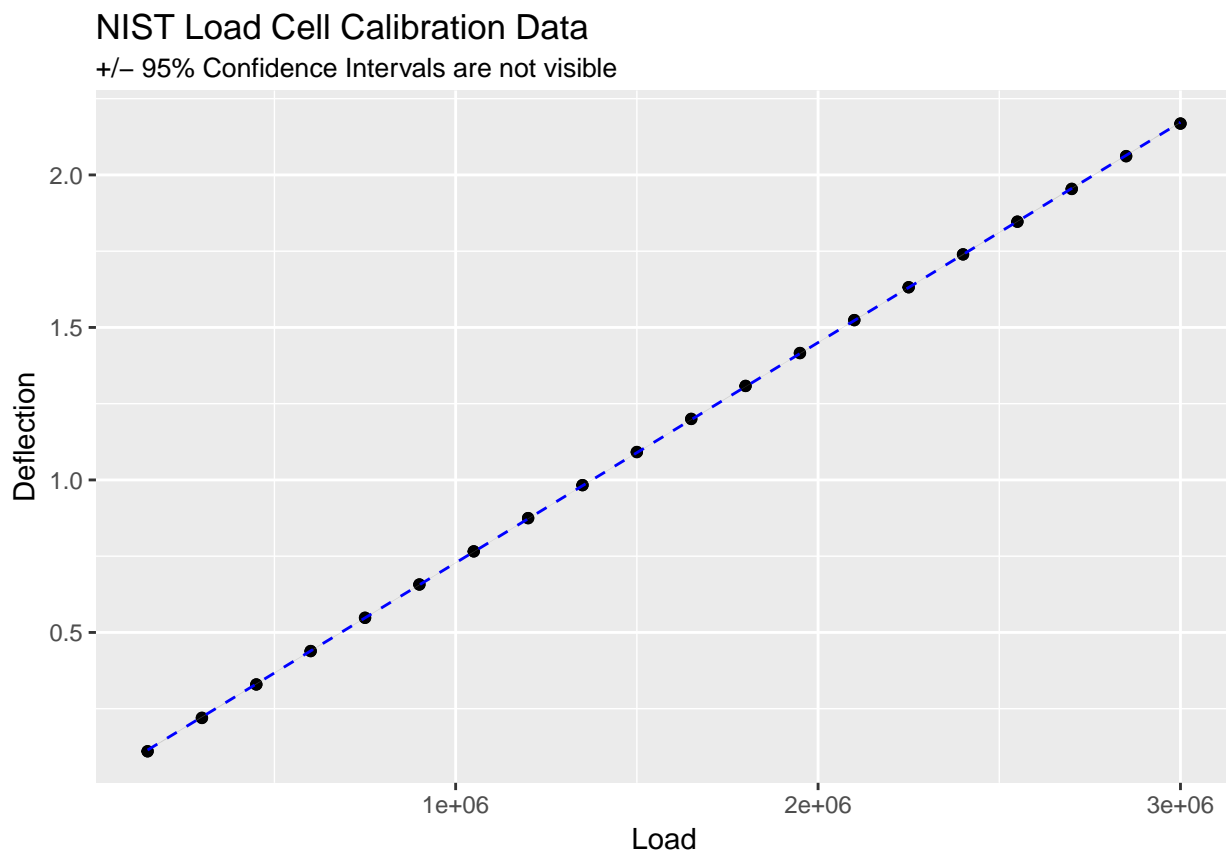
```

## 14 1.52399 2100000 1.5225651 0.0004016005 0.0014248947 0.03421053
## 15 1.63194 2250000 1.6308805 0.0004354772 0.0010595075 0.04022556
## 16 1.73947 2400000 1.7391959 0.0004744336 0.0002741203 0.04774436
## 17 1.84646 2550000 1.8475113 0.0005173233 -0.0010512669 0.05676692
## 18 1.95392 2700000 1.9558267 0.0005632485 -0.0019066541 0.06729323
## 19 2.06128 2850000 2.0641420 0.0006115258 -0.0028620414 0.07932331
## 20 2.16844 3000000 2.1724574 0.0006616404 -0.0040174286 0.09285714
## 21 0.11052 150000 0.1144651 0.0006616404 -0.0039450714 0.09285714
## 22 0.22018 300000 0.2227805 0.0006115258 -0.0026004586 0.07932331
## 23 0.32939 450000 0.3310958 0.0005632485 -0.0017058459 0.06729323
## 24 0.43886 600000 0.4394112 0.0005173233 -0.0005512331 0.05676692
## 25 0.54798 750000 0.5477266 0.0004744336 0.0002533797 0.04774436
## 26 0.65739 900000 0.6560420 0.0004354772 0.0013479925 0.04022556
## 27 0.76596 1050000 0.7643574 0.0004016005 0.0016026053 0.03421053
## 28 0.87474 1200000 0.8726728 0.0003741856 0.0020672180 0.02969925
## 29 0.98300 1350000 0.9809882 0.0003547339 0.0020118308 0.02669173
## 30 1.09150 1500000 1.0893036 0.0003445966 0.0021964436 0.02518797
## 31 1.20004 1650000 1.1976189 0.0003445966 0.0024210564 0.02518797
## 32 1.30818 1800000 1.3059343 0.0003547339 0.0022456692 0.02669173
## 33 1.41613 1950000 1.4142497 0.0003741856 0.0018802820 0.02969925
## 34 1.52408 2100000 1.5225651 0.0004016005 0.0015148947 0.03421053
## 35 1.63159 2250000 1.6308805 0.0004354772 0.0007095075 0.04022556
## 36 1.73965 2400000 1.7391959 0.0004744336 0.0004541203 0.04774436
## 37 1.84696 2550000 1.8475113 0.0005173233 -0.0005512669 0.05676692
## 38 1.95445 2700000 1.9558267 0.0005632485 -0.0013766541 0.06729323
## 39 2.06177 2850000 2.0641420 0.0006115258 -0.0023720414 0.07932331
## 40 2.16829 3000000 2.1724574 0.0006616404 -0.0041674286 0.09285714
##      .sigma      .cooksd .std.resid
## 1 0.002073000 0.2187217636 -2.0672413
## 2 0.002130114 0.1029350494 -1.5457875
## 3 0.002183373 0.0211558343 -0.7658028
## 4 0.002199263 0.0012007249 -0.1997554
## 5 0.002199825 0.0005139600 0.1431843
## 6 0.002195253 0.0037346550 0.4221568
## 7 0.002190258 0.0062011368 0.5917142
## 8 0.002169647 0.0161517779 1.0273197
## 9 0.002176743 0.0111520670 0.9018401
## 10 0.002170924 0.0130728091 1.0059197
## 11 0.002164101 0.0160720896 1.1153599
## 12 0.002167204 0.0156114747 1.0670231
## 13 0.002181165 0.0101324217 0.8136771
## 14 0.002187470 0.0078977192 0.6677705
## 15 0.002193224 0.0051989205 0.4980869
## 16 0.002199934 0.0004196031 0.1293749
## 17 0.002193211 0.0074786732 -0.4985275
## 18 0.002176350 0.0298240268 -0.9092535
## 19 0.002145083 0.0812979572 -1.3737509
## 20 0.002088296 0.1931530525 -1.9426563
## 21 0.002092402 0.1862580234 -1.9076675
## 22 0.002154838 0.0671162569 -1.2481938
## 23 0.002181174 0.0238727261 -0.8134912
## 24 0.002198439 0.0020562178 -0.2614035
## 25 0.002200004 0.0003585089 0.1195861
## 26 0.002188761 0.0084155020 0.6337070

```

```
## 27 0.002184026 0.0099905466 0.7510537
## 28 0.002173203 0.0142970553 0.9665376
## 29 0.002174730 0.0120948393 0.9391866
## 30 0.002169812 0.0135622837 1.0245786
## 31 0.002163176 0.0164779249 1.1293541
## 32 0.002168365 0.0150698435 1.0483498
## 33 0.002177927 0.0118282359 0.8791347
## 34 0.002185777 0.0089269075 0.7099485
## 35 0.002197195 0.0023314123 0.3335478
## 36 0.002199088 0.0011515906 0.2143284
## 37 0.002198439 0.0020564702 -0.2614196
## 38 0.002187904 0.0155479140 -0.6565048
## 39 0.002162561 0.0558434622 -1.1385558
## 40 0.002079520 0.2078459555 -2.0151899
```

```
ggplot(load_cell, aes(Load, Deflection)) +
  geom_point() +
  stat_smooth(method = lm, linetype = "dashed", colour = "blue", size = 0.5) +
  ggtitle("NIST Load Cell Calibration Data", subtitle = "+/- 95% Confidence Intervals are not visible")
```



#### 4.3.1.2 But wait! What about the residuals?

```
load_cell_resid = resid(load_cell_model)
load_cell_resid
```

```
##          1          2          3          4          5
```

```
## -0.0042750714 -0.0032204586 -0.0016058459 -0.0004212331 0.0003033797
##          6          7          8          9          10
## 0.0008979925 0.0012626053 0.0021972180 0.0019318308 0.0021564436
##          11          12          13          14          15
## 0.0023910564 0.0022856692 0.0017402820 0.0014248947 0.0010595075
##          16          17          18          19          20
## 0.0002741203 -0.0010512669 -0.0019066541 -0.0028620414 -0.0040174286
##          21          22          23          24          25
## -0.0039450714 -0.0026004586 -0.0017058459 -0.0005512331 0.0002533797
##          26          27          28          29          30
## 0.0013479925 0.0016026053 0.0020672180 0.0020118308 0.0021964436
##          31          32          33          34          35
## 0.0024210564 0.0022456692 0.0018802820 0.0015148947 0.0007095075
##          36          37          38          39          40
## 0.0004541203 -0.0005512669 -0.0013766541 -0.0023720414 -0.0041674286

# ggplot() +
#   geom_point(aes(LoadCell$Load, LC.resid)) +
#   geom_hline(aes(yintercept=0)) +
#   geom_hline(aes(yintercept=+2*(summary(m.LC)$sigma)), linetype = "dashed") +
#   geom_hline(aes(yintercept=-2*(summary(m.LC)$sigma)), linetype = "dashed") +
#   ggtitle("Deflection Load Residuals", subtitle = "+/- 2(Residual Statndard Deviation)") +
#   theme(plot.title = element_text(hjust = 0.5), plot.subtitle = element_text(hjust = 0.5))
```

Using the `augment()` function we can plot the residuals very easily

```
load_cell_fit <- augment(load_cell_model)
load_cell_fit
```

	Deflection	Load	.fitted	.se.fit	.resid	.hat
## 1	0.11019	150000	0.1144651	0.0006616404	-0.0042750714	0.09285714
## 2	0.21956	300000	0.2227805	0.0006115258	-0.0032204586	0.07932331
## 3	0.32949	450000	0.3310958	0.0005632485	-0.0016058459	0.06729323
## 4	0.43899	600000	0.4394112	0.0005173233	-0.0004212331	0.05676692
## 5	0.54803	750000	0.5477266	0.0004744336	0.0003033797	0.04774436
## 6	0.65694	900000	0.6560420	0.0004354772	0.0008979925	0.04022556
## 7	0.76562	1050000	0.7643574	0.0004016005	0.0012626053	0.03421053
## 8	0.87487	1200000	0.8726728	0.0003741856	0.0021972180	0.02969925
## 9	0.98292	1350000	0.9809882	0.0003547339	0.0019318308	0.02669173
## 10	1.09146	1500000	1.0893036	0.0003445966	0.0021564436	0.02518797
## 11	1.20001	1650000	1.1976189	0.0003445966	0.0023910564	0.02518797
## 12	1.30822	1800000	1.3059343	0.0003547339	0.0022856692	0.02669173
## 13	1.41599	1950000	1.4142497	0.0003741856	0.0017402820	0.02969925
## 14	1.52399	2100000	1.5225651	0.0004016005	0.0014248947	0.03421053
## 15	1.63194	2250000	1.6308805	0.0004354772	0.0010595075	0.04022556
## 16	1.73947	2400000	1.7391959	0.0004744336	0.0002741203	0.04774436
## 17	1.84646	2550000	1.8475113	0.0005173233	-0.0010512669	0.05676692
## 18	1.95392	2700000	1.9558267	0.0005632485	-0.0019066541	0.06729323
## 19	2.06128	2850000	2.0641420	0.0006115258	-0.0028620414	0.07932331
## 20	2.16844	3000000	2.1724574	0.0006616404	-0.0040174286	0.09285714
## 21	0.11052	150000	0.1144651	0.0006616404	-0.0039450714	0.09285714
## 22	0.22018	300000	0.2227805	0.0006115258	-0.0026004586	0.07932331
## 23	0.32939	450000	0.3310958	0.0005632485	-0.0017058459	0.06729323
## 24	0.43886	600000	0.4394112	0.0005173233	-0.0005512331	0.05676692
## 25	0.54798	750000	0.5477266	0.0004744336	0.0002533797	0.04774436



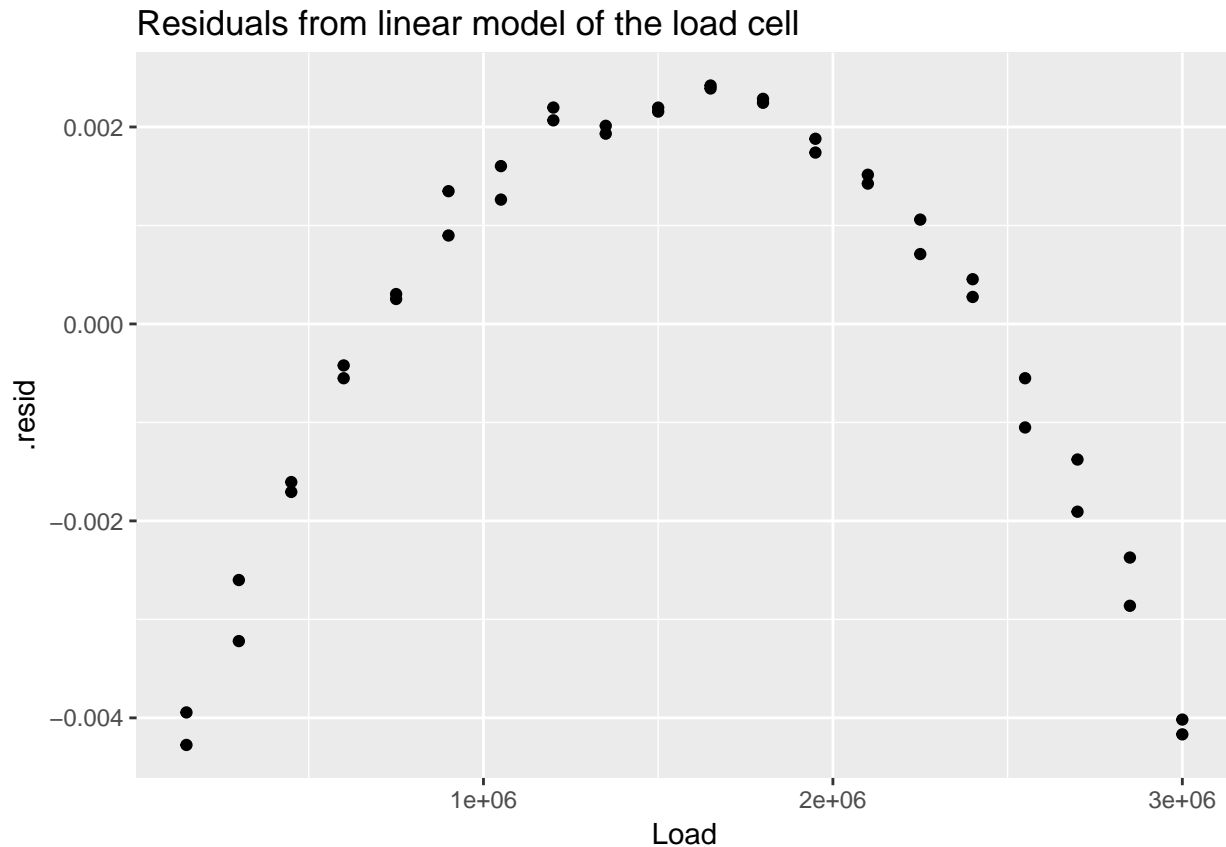
```

## 26    0.65739  900000  0.6560420  0.0004354772  0.0013479925  0.04022556
## 27    0.76596 1050000  0.7643574  0.0004016005  0.0016026053  0.03421053
## 28    0.87474 1200000  0.8726728  0.0003741856  0.0020672180  0.02969925
## 29    0.98300 1350000  0.9809882  0.0003547339  0.0020118308  0.02669173
## 30    1.09150 1500000  1.0893036  0.0003445966  0.0021964436  0.02518797
## 31    1.20004 1650000  1.1976189  0.0003445966  0.0024210564  0.02518797
## 32    1.30818 1800000  1.3059343  0.0003547339  0.0022456692  0.02669173
## 33    1.41613 1950000  1.4142497  0.0003741856  0.0018802820  0.02969925
## 34    1.52408 2100000  1.5225651  0.0004016005  0.0015148947  0.03421053
## 35    1.63159 2250000  1.6308805  0.0004354772  0.0007095075  0.04022556
## 36    1.73965 2400000  1.7391959  0.0004744336  0.0004541203  0.04774436
## 37    1.84696 2550000  1.8475113  0.0005173233 -0.0005512669  0.05676692
## 38    1.95445 2700000  1.9558267  0.0005632485 -0.0013766541  0.06729323
## 39    2.06177 2850000  2.0641420  0.0006115258 -0.0023720414  0.07932331
## 40    2.16829 3000000  2.1724574  0.0006616404 -0.0041674286  0.09285714
##      .sigma      .cooks d .std.resid
## 1  0.002073000  0.2187217636 -2.0672413
## 2  0.002130114  0.1029350494 -1.5457875
## 3  0.002183373  0.0211558343 -0.7658028
## 4  0.002199263  0.0012007249 -0.1997554
## 5  0.002199825  0.0005139600  0.1431843
## 6  0.002195253  0.0037346550  0.4221568
## 7  0.002190258  0.0062011368  0.5917142
## 8  0.002169647  0.0161517779  1.0273197
## 9  0.002176743  0.0111520670  0.9018401
## 10 0.002170924  0.0130728091  1.0059197
## 11 0.002164101  0.0160720896  1.1153599
## 12 0.002167204  0.0156114747  1.0670231
## 13 0.002181165  0.0101324217  0.8136771
## 14 0.002187470  0.0078977192  0.6677705
## 15 0.002193224  0.0051989205  0.4980869
## 16 0.002199934  0.0004196031  0.1293749
## 17 0.002193211  0.0074786732 -0.4985275
## 18 0.002176350  0.0298240268 -0.9092535
## 19 0.002145083  0.0812979572 -1.3737509
## 20 0.002088296  0.1931530525 -1.9426563
## 21 0.002092402  0.1862580234 -1.9076675
## 22 0.002154838  0.0671162569 -1.2481938
## 23 0.002181174  0.0238727261 -0.8134912
## 24 0.002198439  0.0020562178 -0.2614035
## 25 0.002200004  0.0003585089  0.1195861
## 26 0.002188761  0.0084155020  0.6337070
## 27 0.002184026  0.0099905466  0.7510537
## 28 0.002173203  0.0142970553  0.9665376
## 29 0.002174730  0.0120948393  0.9391866
## 30 0.002169812  0.0135622837  1.0245786
## 31 0.002163176  0.0164779249  1.1293541
## 32 0.002168365  0.0150698435  1.0483498
## 33 0.002177927  0.0118282359  0.8791347
## 34 0.002185777  0.0089269075  0.7099485
## 35 0.002197195  0.0023314123  0.3335478
## 36 0.002199088  0.0011515906  0.2143284
## 37 0.002198439  0.0020564702 -0.2614196
## 38 0.002187904  0.0155479140 -0.6565048

```

```
## 39 0.002162561 0.0558434622 -1.1385558
## 40 0.002079520 0.2078459555 -2.0151899
```

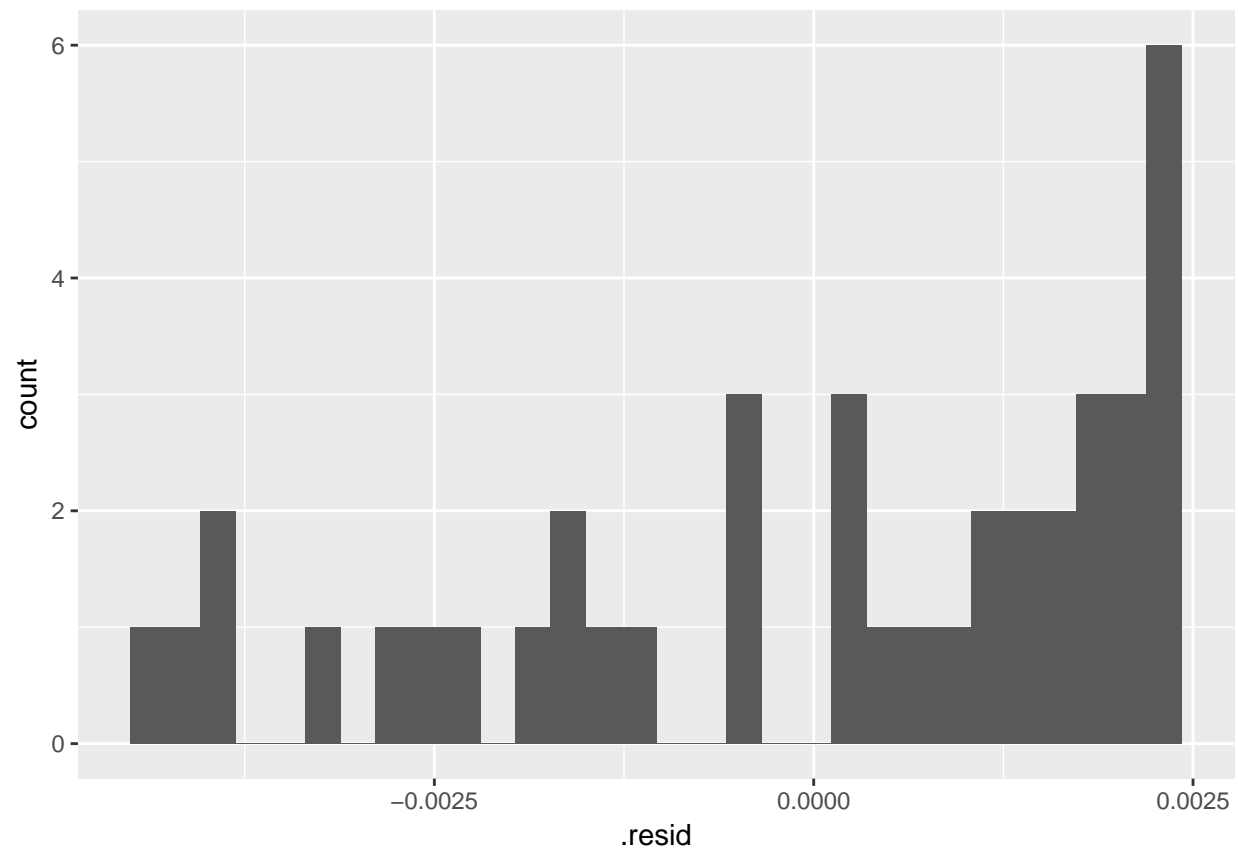
```
ggplot(load_cell_fit) +
  geom_point(aes(Load, .resid)) +
  ggtitle("Residuals from linear model of the load cell")
```



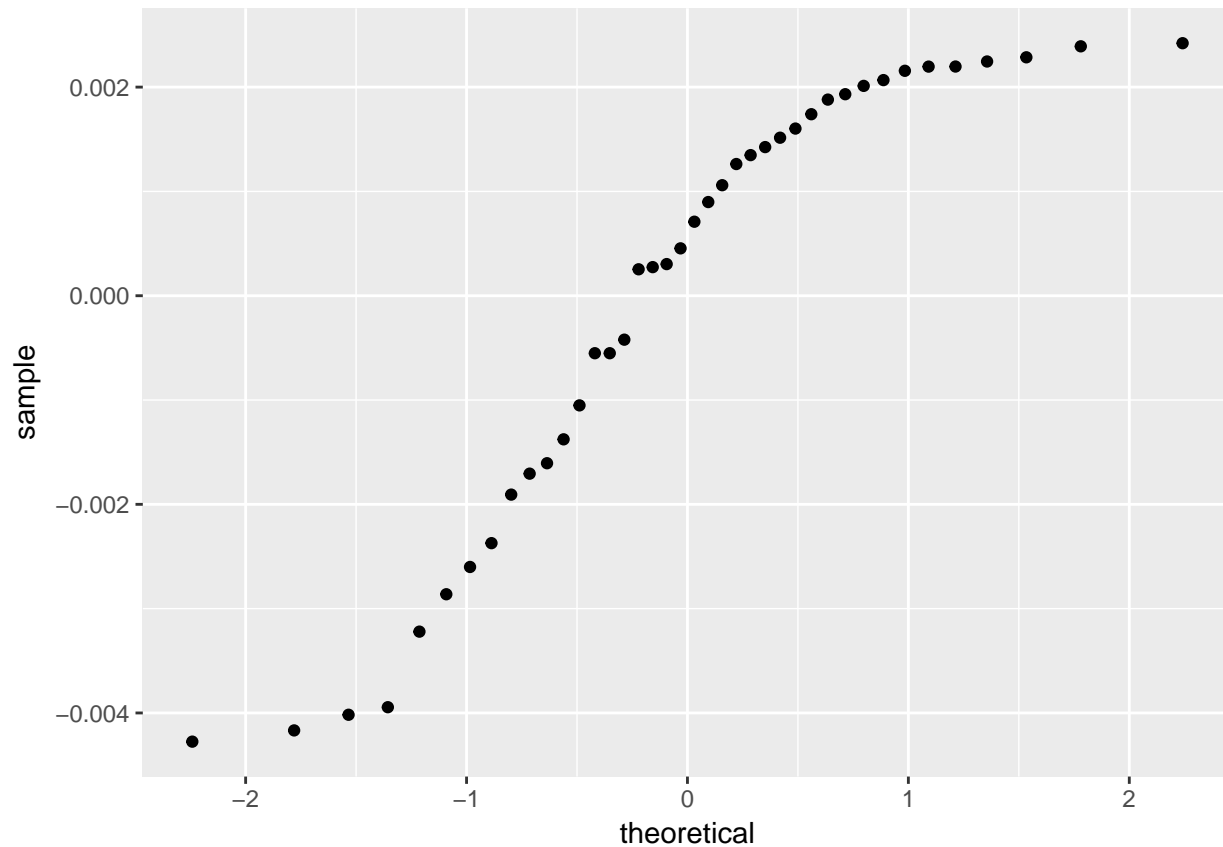
The residuals from a good model would be random. Although not necessary, we can plot a histogram or qqplot to demonstrate the residuals are not following a normal distribution.

```
ggplot(load_cell_fit) +
  geom_histogram(aes(.resid))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(load_cell_fit) +  
  geom_qq(aes(sample = .resid))
```



#### 4.3.1.3 Model Refinement

$$D = \beta_0 + \beta_1 L + \beta_2 L^2 + \varepsilon$$

We can use the linear model function, `lm()`, by creating a new variable  $L^2$ .

```
load_cell_2 <- mutate(load_cell, Load_squared = Load^2)
load_cell_2
```

```
## # A tibble: 40 x 3
##   Deflection    Load Load_squared
##   <dbl>    <dbl>    <dbl>
## 1    0.110  150000.    2.25e10
## 2    0.220  300000.    9.00e10
## 3    0.329  450000.    2.02e11
## 4    0.439  600000.    3.60e11
## 5    0.548  750000.    5.62e11
## 6    0.657  900000.    8.10e11
## 7    0.766 1050000.    1.10e12
## 8    0.875 1200000.    1.44e12
## 9    0.983 1350000.    1.82e12
## 10   1.09 1500000.    2.25e12
## # ... with 30 more rows
```

```
load_cell_model_2 <- lm(Deflection ~ Load + Load_squared, load_cell_2)
summary(load_cell_model_2)
```

```
##
## Call:
## lm(formula = Deflection ~ Load + Load_squared, data = load_cell_2)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.468e-04 -1.578e-04  3.817e-05  1.088e-04  4.235e-04
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  6.736e-04  1.079e-04   6.24 2.97e-07 ***
## Load        7.321e-07  1.578e-10 4638.65 < 2e-16 ***
## Load_squared -3.161e-15  4.867e-17  -64.95 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0002052 on 37 degrees of freedom
## Multiple R-squared:  1, Adjusted R-squared:  1
## F-statistic: 1.853e+08 on 2 and 37 DF, p-value: < 2.2e-16

load_cell_fit_2 <- augment(load_cell_model_2)
load_cell_fit_2
```

	Deflection	Load	Load_squared	.fitted	.se.fit	.resid
## 1	0.11019	150000	2.2500e+10	0.1104113	8.834303e-05	-2.213214e-04
## 2	0.21956	300000	9.0000e+10	0.2200068	7.185366e-05	-4.468402e-04
## 3	0.32949	450000	2.0250e+11	0.3294601	5.888246e-05	2.987782e-05
## 4	0.43899	600000	3.6000e+11	0.4387712	4.986859e-05	2.188327e-04
## 5	0.54803	750000	5.6250e+11	0.5479400	4.495244e-05	9.002444e-05
## 6	0.65694	900000	8.1000e+11	0.6569665	4.354343e-05	-2.654699e-05
## 7	0.76562	1050000	1.1025e+12	0.7658509	4.437259e-05	-2.308816e-04
## 8	0.87487	1200000	1.4400e+12	0.8745930	4.609026e-05	2.770207e-04
## 9	0.98292	1350000	1.8225e+12	0.9831928	4.770597e-05	-2.728402e-04
## 10	1.09146	1500000	2.2500e+12	1.0916505	4.864177e-05	-1.904643e-04
## 11	1.20001	1650000	2.7225e+12	1.1999659	4.864177e-05	4.414850e-05
## 12	1.30822	1800000	3.2400e+12	1.3081390	4.770597e-05	8.099812e-05
## 13	1.41599	1950000	3.8025e+12	1.4161699	4.609026e-05	-1.799154e-04
## 14	1.52399	2100000	4.4100e+12	1.5240586	4.437259e-05	-6.859211e-05
## 15	1.63194	2250000	5.0625e+12	1.6318050	4.354343e-05	1.349680e-04
## 16	1.73947	2400000	5.7600e+12	1.7394092	4.495244e-05	6.076504e-05
## 17	1.84646	2550000	6.5025e+12	1.8468712	4.986859e-05	-4.112011e-04
## 18	1.95392	2700000	7.2900e+12	1.9541909	5.888246e-05	-2.709305e-04
## 19	2.06128	2850000	8.1225e+12	2.0613684	7.185366e-05	-8.842293e-05
## 20	2.16844	3000000	9.0000e+12	2.1684037	8.834303e-05	3.632143e-05
## 21	0.11052	150000	2.2500e+10	0.1104113	8.834303e-05	1.086786e-04
## 22	0.22018	300000	9.0000e+10	0.2200068	7.185366e-05	1.731598e-04
## 23	0.32939	450000	2.0250e+11	0.3294601	5.888246e-05	-7.012218e-05
## 24	0.43886	600000	3.6000e+11	0.4387712	4.986859e-05	8.883271e-05
## 25	0.54798	750000	5.6250e+11	0.5479400	4.495244e-05	4.002444e-05
## 26	0.65739	900000	8.1000e+11	0.6569665	4.354343e-05	4.234530e-04
## 27	0.76596	1050000	1.1025e+12	0.7658509	4.437259e-05	1.091184e-04
## 28	0.87474	1200000	1.4400e+12	0.8745930	4.609026e-05	1.470207e-04
## 29	0.98300	1350000	1.8225e+12	0.9831928	4.770597e-05	-1.928402e-04
## 30	1.09150	1500000	2.2500e+12	1.0916505	4.864177e-05	-1.504643e-04
## 31	1.20004	1650000	2.7225e+12	1.1999659	4.864177e-05	7.414850e-05

```

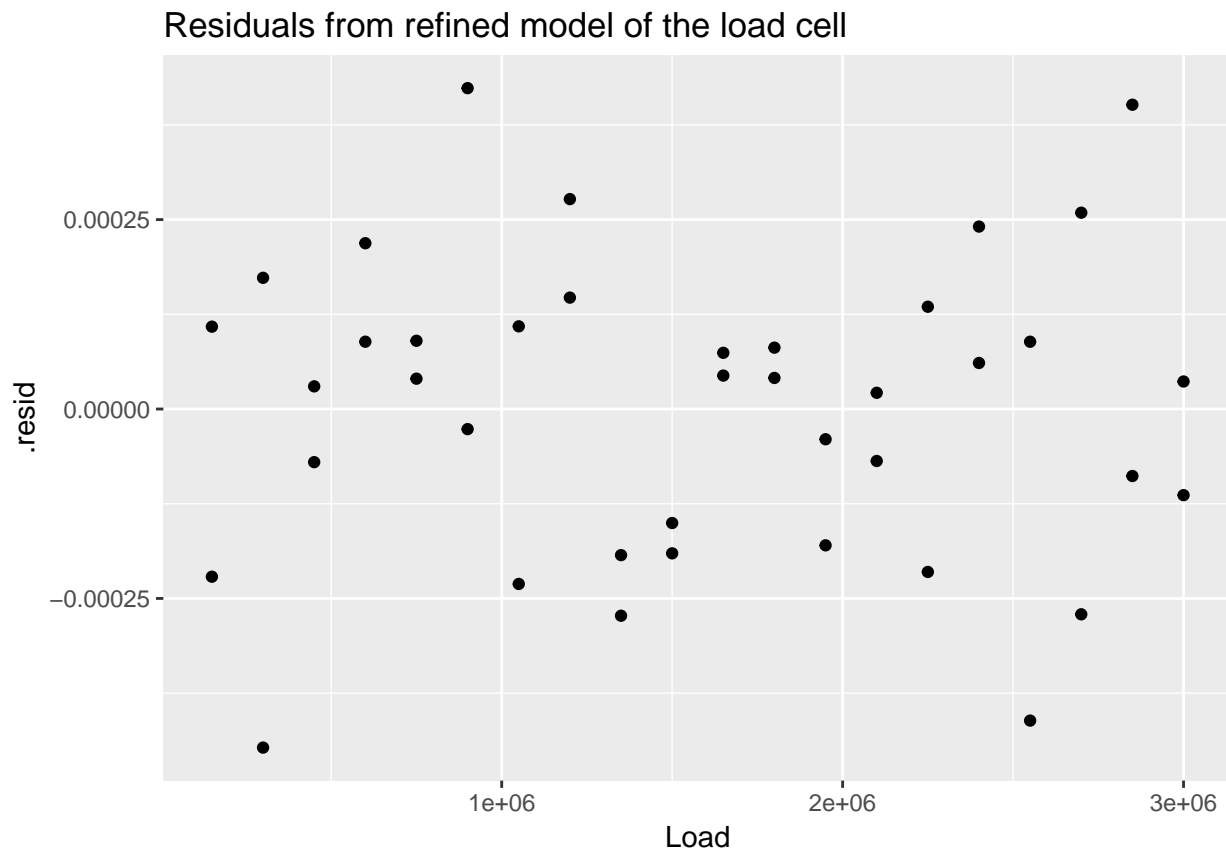
## 32    1.30818 1800000    3.2400e+12 1.3081390 4.770597e-05 4.099812e-05
## 33    1.41613 1950000    3.8025e+12 1.4161699 4.609026e-05 -3.991541e-05
## 34    1.52408 2100000    4.4100e+12 1.5240586 4.437259e-05 2.140789e-05
## 35    1.63159 2250000    5.0625e+12 1.6318050 4.354343e-05 -2.150320e-04
## 36    1.73965 2400000    5.7600e+12 1.7394092 4.495244e-05 2.407650e-04
## 37    1.84696 2550000    6.5025e+12 1.8468712 4.986859e-05 8.879887e-05
## 38    1.95445 2700000    7.2900e+12 1.9541909 5.888246e-05 2.590695e-04
## 39    2.06177 2850000    8.1225e+12 2.0613684 7.185366e-05 4.015771e-04
## 40    2.16829 3000000    9.0000e+12 2.1684037 8.834303e-05 -1.136786e-04
##      .hat      .sigma      .cooksd .std.resid
## 1  0.18538961 0.0002039531 0.1083557670 -1.1951404
## 2  0.12264183 0.0001922123 0.2518888277 -2.3250603
## 3  0.08235931 0.0002079426 0.0006913290 0.1520138
## 4  0.05907382 0.0002045811 0.0253004370 1.0995244
## 5  0.04800068 0.0002074384 0.0033987136 0.4496893
## 6  0.04503873 0.0002079583 0.0002755909 -0.1324015
## 7  0.04677033 0.0002042395 0.0217256885 -1.1525531
## 8  0.05046138 0.0002025394 0.0340077449 1.3855631
## 9  0.05406129 0.0002026849 0.0356120360 -1.3672481
## 10 0.05620301 0.0002054251 0.0181237925 -0.9555308
## 11 0.05620301 0.0002078697 0.0009737642 0.2214864
## 12 0.05406129 0.0002075440 0.0031385560 0.4058952
## 13 0.05046138 0.0002057188 0.0143446582 -0.8998756
## 14 0.04677033 0.0002076778 0.0019175348 -0.3424095
## 15 0.04503873 0.0002067300 0.0071235449 0.6731448
## 16 0.04800068 0.0002077485 0.0015484646 0.3035330
## 17 0.05907382 0.0001956411 0.0893330479 -2.0660791
## 18 0.08235931 0.0002025961 0.0568463516 -1.3784528
## 19 0.12264183 0.0002074117 0.0098635717 -0.4600943
## 20 0.18538961 0.0002078994 0.0029183068 0.1961365
## 21 0.18538961 0.0002070372 0.0261272044 0.5868666
## 22 0.12264183 0.0002057130 0.0378266955 0.9010087
## 23 0.08235931 0.0002076495 0.0038080074 -0.3567710
## 24 0.05907382 0.0002074468 0.0041691675 0.4463397
## 25 0.04800068 0.0002078952 0.0006718065 0.1999297
## 26 0.04503873 0.0001950675 0.0701204501 2.1119458
## 27 0.04677033 0.0002071719 0.0048527858 0.5447155
## 28 0.05046138 0.0002064820 0.0095787822 0.7353473
## 29 0.05406129 0.0002053659 0.0177899720 -0.9663547
## 30 0.05620301 0.0002063997 0.0113106830 -0.7548568
## 31 0.05620301 0.0002076183 0.0027467977 0.3719919
## 32 0.05406129 0.0002078889 0.0008040960 0.2054485
## 33 0.05046138 0.0002078955 0.0007060488 -0.1996433
## 34 0.04677033 0.0002079755 0.0001867854 0.1068675
## 35 0.04503873 0.0002047490 0.0180817416 -1.0724586
## 36 0.04800068 0.0002039013 0.0243097555 1.2026674
## 37 0.05907382 0.0002074473 0.0041659922 0.4461697
## 38 0.08235931 0.0002030652 0.0519780155 1.3181064
## 39 0.12264183 0.0001953495 0.2034427365 2.0895409
## 40 0.18538961 0.0002069456 0.0285865876 -0.6138667

```

```

ggplot(load_cell_fit_2) +
  geom_point(aes(Load, .resid)) +
  ggtitle("Residuals from refined model of the load cell")

```



#### 4.3.1.3.1 Could we have used a non-linear least squares fit model?

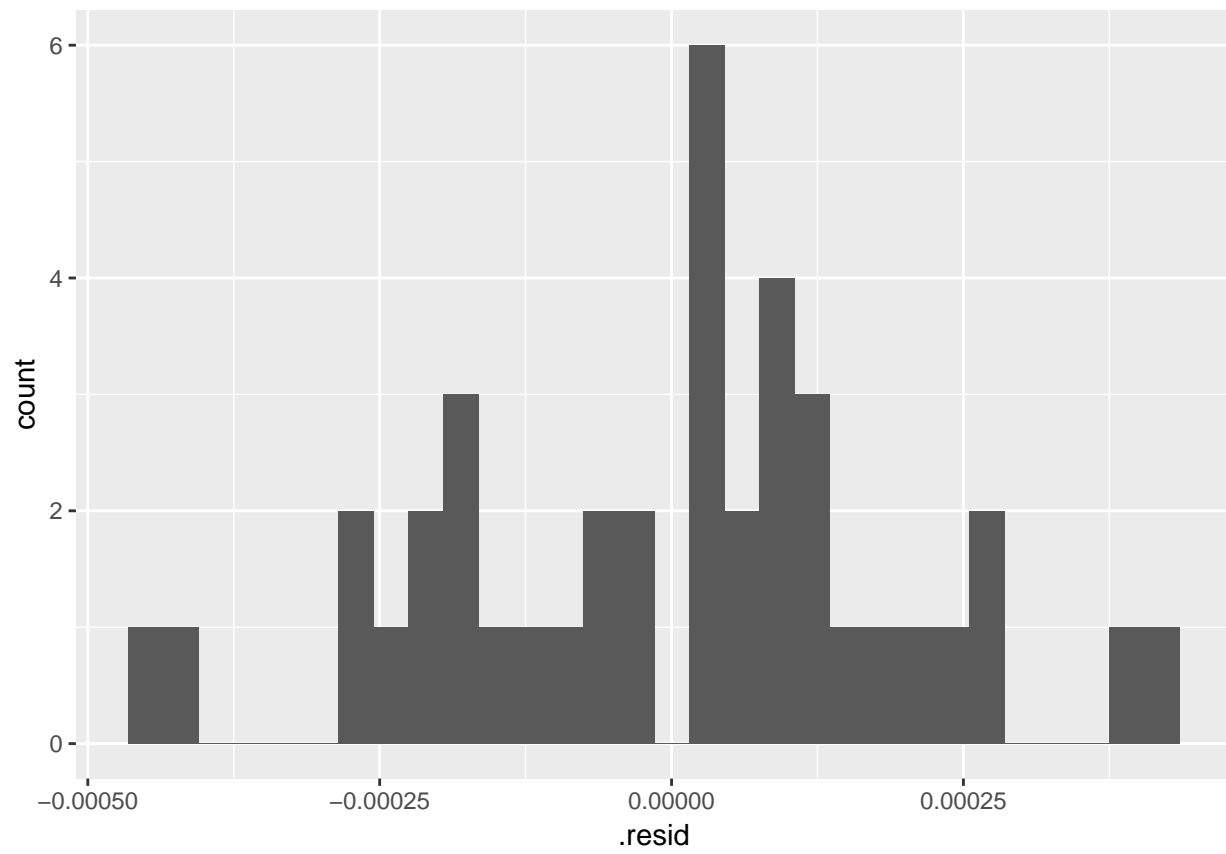
```
load_cell_model_3 <- nls(Deflection ~ b0 + b1*Load + b2*Load^2, load_cell_2, start = c(b0 = 0, b1 = 0, b2 = 0))
summary(load_cell_model_3)
```

```
##
## Formula: Deflection ~ b0 + b1 * Load + b2 * Load^2
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## b0  6.736e-04  1.079e-04   6.24 2.97e-07 ***
## b1  7.321e-07  1.578e-10 4638.65 < 2e-16 ***
## b2 -3.161e-15  4.867e-17 -64.95 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0002052 on 37 degrees of freedom
##
## Number of iterations to convergence: 1
## Achieved convergence tolerance: 1.328e-06
```

The results are identical.

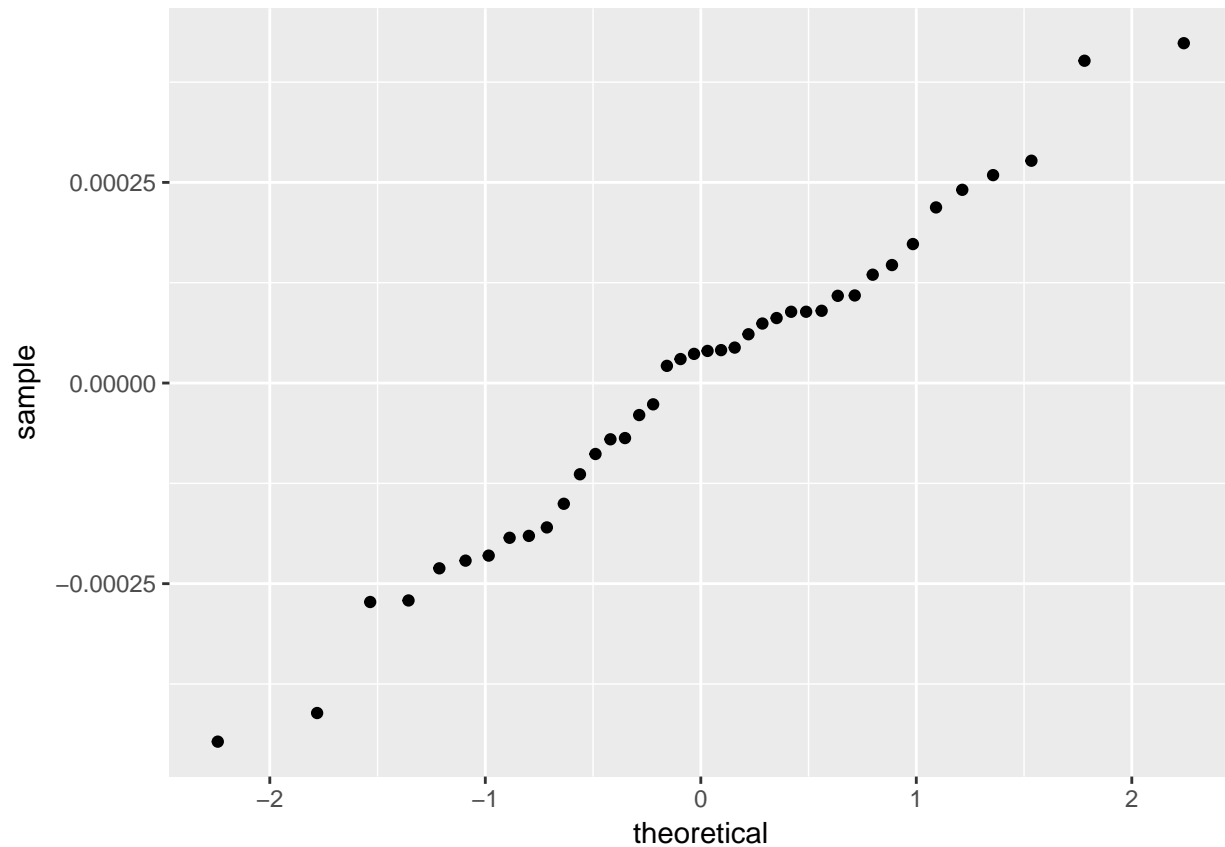
```
ggplot(load_cell_fit_2) +
  geom_histogram(aes(.resid))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(load_cell_fit_2) +  
  geom_qq(aes(sample = .resid))
```





### 4.3.2 Thermal expansion of copper

from section 4.6.4. Thermal Expansion of Copper Case Study

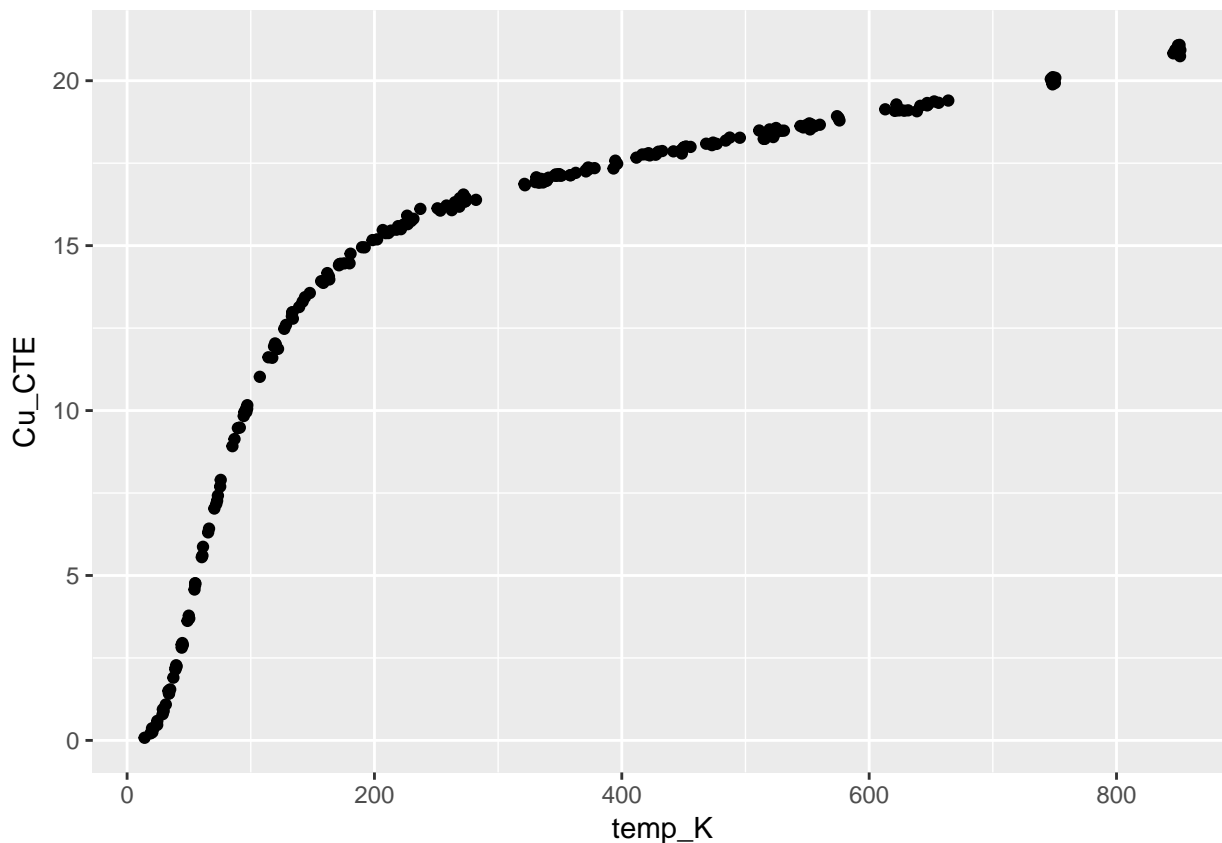
This case study illustrates the use of a class of nonlinear models called rational function models. The data set used is the thermal expansion of copper related to temperature.

```
CTECu <- read_table2(
  "NIST data/HAHN1.dat", skip = 25, col_names = FALSE)
```

```
## Parsed with column specification:
## cols(
##   X1 = col_double(),
##   X2 = col_double()
## )
```

```
CTECu <- CTECu %>%
  rename(temp_K = X1, Cu_CTE = X2)
View(CTECu)
```

```
ggplot(CTECu, aes(temp_K, Cu_CTE)) +
  geom_point()
```



### 4.3.3 Quadratic/Quadratic (Q/Q) model

The NIST handbook has a procedure for calculating estimates for the model, below, I just used guess values for the equation

$$y = \frac{(A0 + A1 \cdot x + A2 \cdot x^2)}{(1 + B1 \cdot x + B2 \cdot x^2)}$$

```
model_Cu <- nls(Cu_CTE ~ ((a0 + a1*temp_K + a2*temp_K^2)/(1 + b1*temp_K + b2*temp_K^2)),
  CTECu, start = list(a0 = 0, a1 = -1, a2 = -1, b1 = 0, b2 = 0), trace = T)
```

```
## 1.344556e+13 :    0 -1 -1  0  0
## 1697329 :   -3.351400e+00  1.797879e-01 -5.745645e-04  7.915158e-07 -3.877688e-10
## 177589.3 :   -3.319661e+00  1.750319e-01 -3.592189e-04  1.144561e-03 -6.445222e-07
## 32411.82 :   -4.730736e+00  2.146213e-01 -3.235814e-04  3.851759e-03 -2.232626e-06
## 5374.946 :   -6.413603e+00  2.683958e-01 -2.844465e-04  7.799104e-03 -4.266107e-06
## 690.5713 :   -6.901674e+00  2.867489e-01 -1.804611e-04  1.009256e-02 -3.131612e-06
## 217.1164 :   -5.970973e+00  2.481232e-01  1.250216e-04  8.918691e-03  1.150181e-05
## 114.0929 :   -3.145220e+00  1.061122e-01  1.610442e-03  4.783451e-03  8.707152e-05
## 64.59622 :    3.1477349163 -0.2965983768  0.0078946767  0.0013004690  0.0003974542
## 42.78158 :    9.3230025114 -0.8210512798  0.0188009501  0.0103976361  0.0009147904
## 34.34313 :   11.848742450 -1.098105431  0.025888747  0.024139632  0.001231568
## 33.5614 :   11.838847499 -1.129134608  0.027249383  0.029538247  0.001286009
## 33.55298 :   12.220405792 -1.169396827  0.028259353  0.031296606  0.001332281
## 33.55278 :   11.988150281 -1.149285630  0.027831681  0.030880324  0.001312172
## 33.55273 :   12.165006923 -1.165285413  0.028186412  0.031296535  0.001328754
## 33.55271 :   12.034452089 -1.153533233  0.027926998  0.030997296  0.001316621
```

```
## 33.55269 : 12.131480095 -1.162274660 0.028120094 0.031220657 0.001325652
## 33.55268 : 12.059618930 -1.155801947 0.027977138 0.031055397 0.001318966
## 33.55268 : 12.112946981 -1.160605895 0.028083247 0.031178098 0.001323928
## 33.55268 : 12.073406215 -1.157044238 0.028004583 0.031087151 0.001320249
## 33.55267 : 12.102793316 -1.159691514 0.028063056 0.031154770 0.001322984
## 33.55267 : 12.081046435 -1.157732650 0.028019791 0.031104752 0.001320961
## 33.55267 : 12.097167203 -1.159184809 0.028051866 0.031141839 0.001322461
## 33.55267 : 12.085177311 -1.158104731 0.028028009 0.031114250 0.001321345
## 33.55267 : 12.094068505 -1.158905649 0.028045699 0.031134704 0.001322172
## 33.55267 : 12.087436601 -1.158308224 0.028032503 0.031119442 0.001321555
## 33.55267 : 12.092386536 -1.158754113 0.028042351 0.031130832 0.001322016
## 33.55267 : 12.088732963 -1.158425030 0.028035083 0.031122431 0.001321676
## 33.55267 : 12.091445289 -1.158669369 0.028040481 0.031128672 0.001321928
## 33.55267 : 12.08942043 -1.15848695 0.02803645 0.03112401 0.00132174
## 33.55267 : 12.090900623 -1.158620261 0.028039395 0.031127413 0.001321877
## 33.55267 : 12.089833503 -1.158524186 0.028037274 0.031124964 0.001321778
## 33.55267 : 12.090620445 -1.158595059 0.028038839 0.031126773 0.001321851
```

```
summary(model_Cu)
```

```
##
## Formula: Cu_CTE ~ ((a0 + a1 * temp_K + a2 * temp_K^2)/(1 + b1 * temp_K +
##      b2 * temp_K^2))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## a0 12.0906204  4.9457268   2.445  0.01525 *
## a1 -1.1585951  0.4459281  -2.598  0.00997 **
## a2  0.0280388  0.0099339   2.823  0.00518 **
## b1  0.0311268  0.0123461   2.521  0.01237 *
## b2  0.0013219  0.0004639   2.849  0.00478 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3811 on 231 degrees of freedom
##
## Number of iterations to convergence: 32
## Achieved convergence tolerance: 8.018e-06
```

```
glance(model_Cu)
```

```
##      sigma isConv      finTol    logLik      AIC      BIC deviance
## 1 0.3811163  TRUE 8.017872e-06 -104.6851 221.3702 242.1532 33.55267
## df.residual
## 1      231
```

```
augment(model_Cu)
```

```
##      temp_K Cu_CTE      .fitted      .resid
## 1    24.41  0.591  0.20263740  0.388362604
## 2    34.82  1.547  1.55799629 -0.010996290
## 3    44.09  2.902  3.13916746 -0.237167465
## 4    45.07  2.894  3.30744524 -0.413445244
## 5    54.98  4.703  4.94210005 -0.239100048
## 6    65.51  6.307  6.48782610 -0.180826097
## 7    70.53  7.030  7.14914778 -0.119147778
```

```
## 8    75.70  7.898  7.78154503  0.116454973
## 9    89.57  9.470  9.25903236  0.210967637
## 10   91.14  9.484  9.40826472  0.075735280
## 11   96.40 10.072  9.88458561  0.187414386
## 12   97.19 10.163  9.95311700  0.209882997
## 13  114.26 11.615 11.26656602  0.348433983
## 14  120.25 12.005 11.66166565  0.343334345
## 15  127.08 12.478 12.07731227  0.400687732
## 16  133.55 12.982 12.44039495  0.541605047
## 17  133.61 12.970 12.44363272  0.526367277
## 18  158.67 13.926 13.62043804  0.305561962
## 19  172.74 14.452 14.15567440  0.296325603
## 20  171.31 14.404 14.10466048  0.299339518
## 21  202.14 15.190 15.06560294  0.124397055
## 22  220.55 15.550 15.52648312  0.023516883
## 23  221.05 15.528 15.53805198 -0.010051982
## 24  221.39 15.499 15.54589234 -0.046892338
## 25  250.99 16.131 16.15515873 -0.024158729
## 26  268.99 16.438 16.46610887 -0.028108874
## 27  271.80 16.387 16.51126548 -0.124265483
## 28  271.97 16.549 16.51397008  0.035029917
## 29  321.31 16.872 17.18698756 -0.314987562
## 30  321.69 16.830 17.19142843 -0.361428433
## 31  330.14 16.926 17.28772364 -0.361723642
## 32  333.03 16.907 17.31961419 -0.412614189
## 33  333.47 16.966 17.32442437 -0.358424366
## 34  340.77 17.060 17.40253947 -0.342539470
## 35  345.65 17.122 17.45304116 -0.331041159
## 36  373.11 17.311 17.71409685 -0.403096846
## 37  373.79 17.355 17.72010437 -0.365104372
## 38  411.82 17.668 18.02623331 -0.358233309
## 39  419.51 17.767 18.08174912 -0.314749116
## 40  421.59 17.803 18.09643544 -0.293435444
## 41  422.02 17.765 18.09945445 -0.334454452
## 42  422.47 17.768 18.10260764 -0.334607642
## 43  422.61 17.736 18.10358734 -0.367587337
## 44  441.75 17.858 18.23197297 -0.373972966
## 45  447.41 17.877 18.26793801 -0.390938005
## 46  448.70 17.912 18.27601424 -0.364014242
## 47  472.89 18.046 18.41967798 -0.373677978
## 48  476.69 18.085 18.44098172 -0.355981723
## 49  522.47 18.291 18.67429455 -0.383294553
## 50  522.62 18.357 18.67499461 -0.317994608
## 51  524.43 18.426 18.68341166 -0.257411661
## 52  546.75 18.584 18.78280566 -0.198805658
## 53  549.53 18.610 18.79464198 -0.184641978
## 54  575.29 18.870 18.89908047 -0.029080472
## 55  576.00 18.795 18.90183163 -0.106831626
## 56  625.55 19.111 19.07892819  0.032071807
## 57   20.15  0.367  0.05976671  0.307233295
## 58   28.78  0.796  0.65887516  0.137124838
## 59   29.57  0.892  0.76317614  0.128823858
## 60   37.41  1.903  1.98987963 -0.086879626
## 61   39.12  2.150  2.28182032 -0.131820319
```

```
## 62  50.24  3.697  4.17855148 -0.481551482
## 63  61.38  5.870  5.90731429 -0.037314289
## 64  66.25  6.421  6.58833329 -0.167333292
## 65  73.42  7.422  7.50855925 -0.086559249
## 66  95.52  9.944  9.80734632  0.136653680
## 67 107.32 11.023 10.76867928  0.254320724
## 68 122.04 11.870 11.77402819  0.095971811
## 69 134.03 12.786 12.46623314  0.319766858
## 70 163.19 14.067 13.80079176  0.266208244
## 71 163.48 13.974 13.81207896  0.161921040
## 72 175.70 14.462 14.25903034  0.202969659
## 73 179.86 14.464 14.39938426  0.064615736
## 74 211.27 15.381 15.30300305  0.077996951
## 75 217.78 15.483 15.46153988  0.021460123
## 76 219.14 15.590 15.49360705  0.096392951
## 77 262.52 16.075 16.35879653 -0.283796530
## 78 268.01 16.347 16.45015753 -0.103157525
## 79 268.62 16.181 16.46009888 -0.279098880
## 80 336.25 16.915 17.35454484 -0.439544844
## 81 337.23 17.003 17.36505255 -0.362052548
## 82 339.33 16.978 17.38737853 -0.409378534
## 83 427.38 17.756 18.13660333 -0.380603334
## 84 428.58 17.808 18.14479952 -0.336799522
## 85 432.68 17.868 18.17247767 -0.304477673
## 86 528.99 18.481 18.70437208 -0.223372077
## 87 531.08 18.486 18.71386351 -0.227863507
## 88 628.34 19.090 19.08809722  0.001902777
## 89 253.24 16.062 16.19621410 -0.134214101
## 90 273.13 16.337 16.53234301 -0.195343011
## 91 273.66 16.345 16.54069023 -0.195690232
## 92 282.10 16.388 16.66974746 -0.281747456
## 93 346.62 17.159 17.46292119 -0.303921190
## 94 347.19 17.116 17.46870293 -0.352702926
## 95 348.78 17.164 17.48473760 -0.320737599
## 96 351.18 17.123 17.50868379 -0.385683795
## 97 450.10 17.979 18.28472932 -0.305729323
## 98 450.35 17.974 18.28628016 -0.312280163
## 99 451.92 18.007 18.29598212 -0.288982125
## 100 455.56 17.993 18.31823099 -0.325230985
## 101 552.22 18.523 18.80598605 -0.282986051
## 102 553.56 18.669 18.81159745 -0.142597449
## 103 555.74 18.617 18.82067084 -0.203670839
## 104 652.59 19.371 19.16459642  0.206403582
## 105 656.20 19.330 19.17551650  0.154483498
## 106  14.13  0.080  0.77348741 -0.693487408
## 107  20.41  0.248  0.05662611  0.191373893
## 108  31.30  1.089  1.00816471  0.080835292
## 109  33.84  1.418  1.39956756  0.018432442
## 110  39.70  2.278  2.38155051 -0.103550513
## 111  48.83  3.624  3.94438216 -0.320382160
## 112  54.50  4.574  4.86657271 -0.292572712
## 113  60.41  5.556  5.76612933 -0.210129333
## 114  72.77  7.267  7.42904396 -0.162043958
## 115  75.25  7.695  7.72838906 -0.033389062
```

```
## 116 86.84 9.136 8.99136369 0.144636308
## 117 94.88 9.959 9.75056787 0.208432127
## 118 96.40 9.957 9.88458561 0.072414386
## 119 117.37 11.600 11.47547190 0.124528102
## 120 139.08 13.138 12.72947330 0.408526704
## 121 147.73 13.564 13.14657103 0.417428974
## 122 158.63 13.871 13.61880392 0.252196080
## 123 161.84 13.994 13.74780396 0.246196039
## 124 192.11 14.947 14.78222963 0.164770366
## 125 206.76 15.473 15.18803137 0.284968629
## 126 209.07 15.379 15.24746384 0.131536163
## 127 213.32 15.455 15.35384680 0.101153203
## 128 226.44 15.908 15.65987906 0.248120943
## 129 237.12 16.114 15.88663535 0.227364654
## 130 330.90 17.071 17.29616030 -0.225160304
## 131 358.72 17.135 17.58196286 -0.446962856
## 132 370.77 17.282 17.69326577 -0.411265769
## 133 372.72 17.368 17.71064206 -0.342642062
## 134 396.24 17.483 17.90752311 -0.424523105
## 135 416.59 17.764 18.06089749 -0.296897490
## 136 484.02 18.185 18.48117310 -0.296173098
## 137 495.47 18.271 18.54167975 -0.270679752
## 138 514.78 18.236 18.63788133 -0.401881325
## 139 515.65 18.237 18.64205311 -0.405053108
## 140 519.47 18.523 18.66021207 -0.137212071
## 141 544.47 18.627 18.77301150 -0.146011498
## 142 560.11 18.665 18.83865465 -0.173654648
## 143 620.77 19.086 19.06303418 0.022965825
## 144 18.97 0.214 0.09784057 0.116159433
## 145 28.93 0.943 0.67826891 0.264731089
## 146 33.91 1.429 1.41076863 0.018231366
## 147 40.03 2.241 2.43840011 -0.197400110
## 148 44.66 2.951 3.23712804 -0.286128037
## 149 49.87 3.782 4.11738756 -0.335387561
## 150 55.16 4.757 4.97031350 -0.213313499
## 151 60.90 5.602 5.83768000 -0.235680001
## 152 72.08 7.169 7.34380175 -0.174801749
## 153 85.15 8.920 8.82027800 0.099721997
## 154 97.06 10.055 9.94189178 0.113108223
## 155 119.63 12.035 11.62215376 0.412846236
## 156 133.27 12.861 12.42525502 0.435744978
## 157 143.84 13.436 12.96400254 0.471997455
## 158 161.91 14.167 13.75056958 0.416430418
## 159 180.67 14.755 14.42607069 0.328929310
## 160 198.44 15.168 14.96397105 0.204028954
## 161 226.86 15.651 15.66915570 -0.018155704
## 162 229.65 15.746 15.73001114 0.015988863
## 163 258.27 16.216 16.28565218 -0.069652183
## 164 273.77 16.445 16.54241898 -0.097418978
## 165 339.15 16.965 17.38547498 -0.420474978
## 166 350.13 17.121 17.49824509 -0.377245093
## 167 362.75 17.206 17.61995849 -0.413958492
## 168 371.03 17.250 17.69559252 -0.445592517
## 169 393.32 17.339 17.88428738 -0.545287384
```

```
## 170 448.53 17.793 18.27495246 -0.481952459
## 171 473.78 18.123 18.42469678 -0.301696776
## 172 511.12 18.490 18.62018208 -0.130182079
## 173 524.70 18.566 18.68466247 -0.118662470
## 174 548.75 18.645 18.79133263 -0.146332628
## 175 551.64 18.706 18.80354911 -0.097549110
## 176 574.02 18.924 18.89414305 0.029856952
## 177 623.86 19.100 19.07333565 0.026664346
## 178 21.46 0.375 0.06146604 0.313533960
## 179 24.33 0.471 0.19669499 0.274305007
## 180 33.43 1.504 1.33435088 0.169649123
## 181 39.22 2.204 2.29899563 -0.094995630
## 182 44.18 2.813 3.15464924 -0.341649241
## 183 55.02 4.765 4.94837488 -0.183374875
## 184 94.33 9.835 9.70136218 0.133637823
## 185 96.44 10.040 9.88807384 0.151926161
## 186 118.82 11.946 11.57006498 0.375935018
## 187 128.48 12.596 12.15828826 0.437711736
## 188 141.94 13.303 12.87190265 0.431097345
## 189 156.92 13.922 13.54830088 0.373699124
## 190 171.65 14.440 14.11685477 0.323145234
## 191 190.00 14.951 14.71932283 0.231677171
## 192 223.26 15.627 15.58863528 0.038364719
## 193 223.88 15.639 15.60266672 0.036333280
## 194 231.50 15.814 15.76964133 0.044358666
## 195 265.05 16.315 16.40132663 -0.086326629
## 196 269.44 16.334 16.47339806 -0.139398063
## 197 271.78 16.430 16.51094709 -0.080947092
## 198 273.46 16.423 16.53754381 -0.114543806
## 199 334.61 17.024 17.33683230 -0.312832301
## 200 339.79 17.009 17.39223463 -0.383234635
## 201 349.52 17.165 17.49215378 -0.327153784
## 202 358.18 17.134 17.57681079 -0.442810793
## 203 377.98 17.349 17.75667290 -0.407672903
## 204 394.77 17.576 17.89586620 -0.319866198
## 205 429.66 17.848 18.15213896 -0.304138963
## 206 468.22 18.090 18.39304523 -0.303045226
## 207 487.27 18.276 18.49862363 -0.222623626
## 208 519.54 18.404 18.66054244 -0.256542438
## 209 523.03 18.519 18.67690613 -0.157906127
## 210 612.99 19.133 19.03665298 0.096347018
## 211 638.59 19.074 19.12111752 -0.047117521
## 212 641.36 19.239 19.12986584 0.109134164
## 213 622.05 19.280 19.06731345 0.212686549
## 214 631.50 19.101 19.09838763 0.002612371
## 215 663.97 19.398 19.19863025 0.199369748
## 216 646.90 19.252 19.14714500 0.104855005
## 217 748.29 19.890 19.41945281 0.470547190
## 218 749.21 20.007 19.42159564 0.585404361
## 219 750.14 19.929 19.42375656 0.505243437
## 220 647.04 19.268 19.14757794 0.120422056
## 221 646.89 19.324 19.14711406 0.176885936
## 222 746.90 20.049 19.41620554 0.632794460
## 223 748.43 20.107 19.41977922 0.687220777
```

```
## 224 747.35 20.062 19.41725810 0.644741900
## 225 749.27 20.065 19.42173521 0.643264790
## 226 647.61 19.286 19.14933879 0.136661207
## 227 747.78 19.972 19.41826273 0.553737271
## 228 750.51 20.088 19.42461484 0.663385162
## 229 851.37 20.743 19.63143059 1.111569415
## 230 845.97 20.830 19.62157695 1.208423055
## 231 847.54 20.935 19.62445443 1.310545566
## 232 849.93 21.035 19.62881490 1.406185103
## 233 851.61 20.930 19.63186569 1.298134306
## 234 849.75 21.074 19.62848733 1.445512673
## 235 850.98 21.085 19.63072302 1.454276977
## 236 848.23 20.935 19.62571577 1.309284225
```

```
tidy(model_Cu)
```

```
##   term      estimate  std.error statistic    p.value
## 1  a0 12.090620445 4.9457267991  2.444660 0.015247600
## 2  a1 -1.158595059 0.4459281342 -2.598165 0.009974985
## 3  a2  0.028038839 0.0099338856  2.822545 0.005179792
## 4  b1  0.031126773 0.0123461159  2.521179 0.012370785
## 5  b2  0.001321851 0.0004639428  2.849169 0.004779119
```

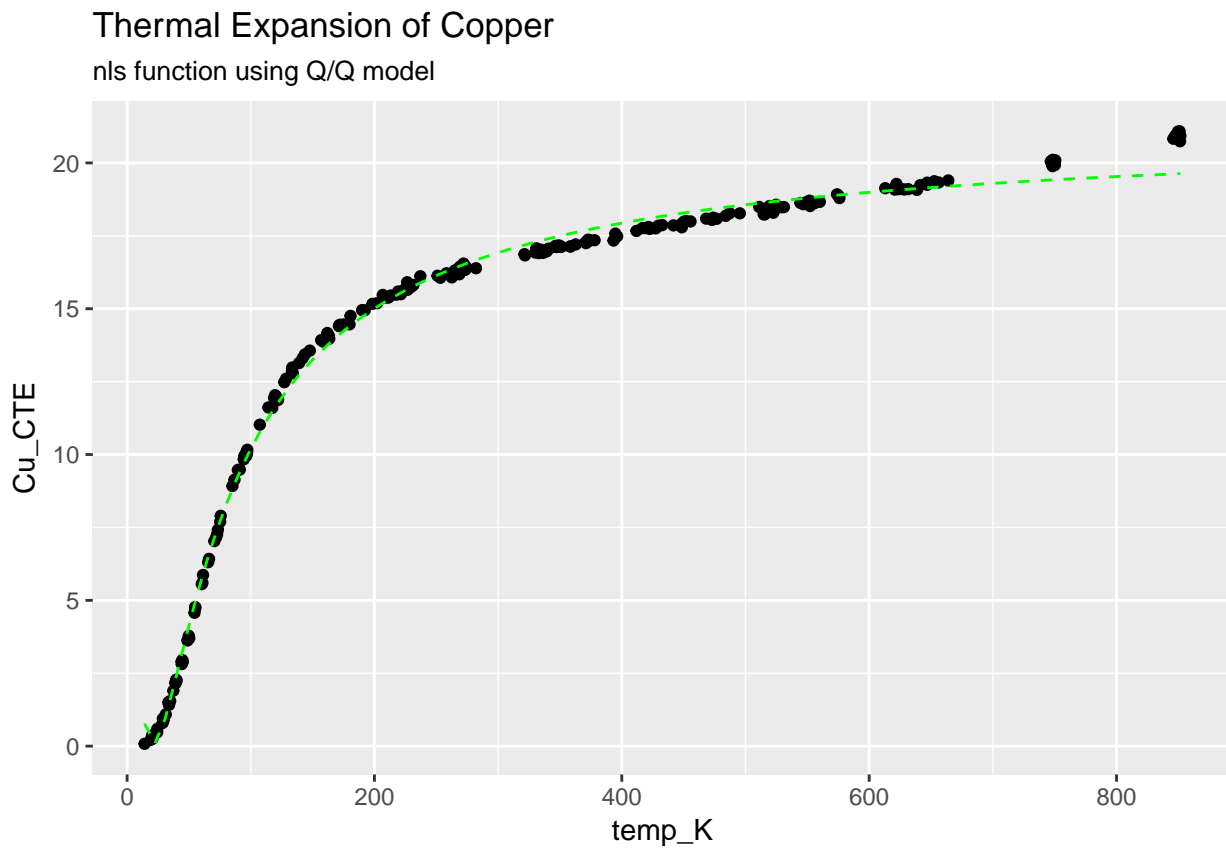
#### 4.3.3.1 Create a function using the fit parameters

```
Cu_fit <- function(x) {
  ((summary(model_Cu)$coefficients[1] + summary(model_Cu)$coefficients[2]*x + summary(model_Cu)$coefficients[3]*x^2))
}
```

#### 4.3.3.2 Add the fitted curve to the graph

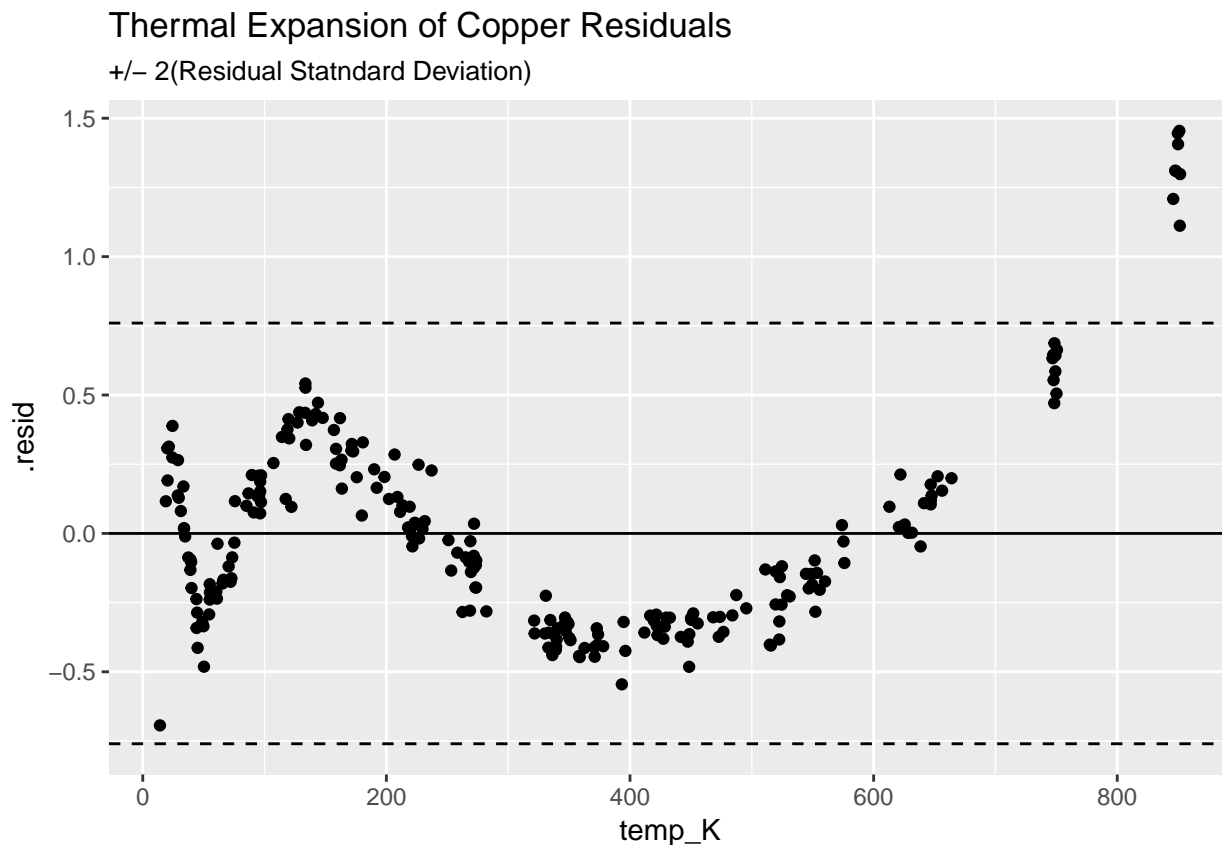
```
ggplot(CTECu, aes(temp_K, Cu_CTE)) +
  geom_point() +
  stat_function(fun = Cu_fit, colour = "green", linetype = "dashed") +
  ggtitle("Thermal Expansion of Copper", subtitle = "nls function using Q/Q model")
```





#### 4.3.3.3 Plot the residulas

```
ggplot(augment(model_Cu)) +
  geom_point(aes(temp_K, .resid)) +
  geom_hline(aes(yintercept=0)) +
  geom_hline(aes(yintercept=+2*(0.38)), linetype = "dashed") +
  geom_hline(aes(yintercept=-2*(0.38)), linetype = "dashed") +
  ggtitle("Thermal Expansion of Copper Residuals", subtitle = "+/- 2(Residual Statndard Deviation)")
```



The fit is not very good, shows a clear structure, and indicates the Q/Q model is insufficient.

#### 4.3.4 Cubic/Cubic Rational Function

$$y = \frac{(A0 + A1 * x + A2x^2 + A3X^3)}{(1 + B1x + B2X^2 + B3X^3)}$$

```
mcc_Cu <- nls(Cu_CTE ~ ((a0 + a1*temp_K + a2*temp_K^2 + a3*temp_K^3)/(1 + b1*temp_K + b2*temp_K^2 + b3*
  CTECu, start = list(a0 = 0, a1 = -1, a2 = -1, a3 = 0, b1 = 0, b2 = 0, b3 = 0),
  trace = T)
```

```
## 1.344556e+13 : 0 -1 -1 0 0 0 0
## 1.339595e+13 : -4.089856e-03 -9.988271e-01 -9.983564e-01 6.676610e-04 -6.676602e-04 -1.055201e-11
## 1.334366e+13 : -4.807459e-03 -9.966232e-01 -9.964072e-01 6.664584e-04 -6.677607e-04 -1.094787e-11
## 1.32396e+13 : -6.863478e-03 -9.922082e-01 -9.925166e-01 6.639777e-04 -6.678813e-04 -1.223912e-11
## 1.30334e+13 : -1.594000e-02 -9.833127e-01 -9.847661e-01 6.593020e-04 -6.683904e-04 -1.602231e-11
## 1.262831e+13 : -6.540076e-02 -9.650849e-01 -9.693885e-01 6.507887e-04 -6.701861e-04 -3.033631e-11
## 1.184743e+13 : -1.788916e-01 -9.289031e-01 -9.391153e-01 6.341455e-04 -6.739522e-04 -6.184747e-11
## 1.040295e+13 : -4.142861e-01 -8.583930e-01 -8.804668e-01 5.994049e-04 -6.790616e-04 -1.428677e-10
## 7.989692e+12 : -9.341122e-01 -7.234575e-01 -7.705432e-01 5.175015e-04 -6.708211e-04 -4.851866e-10
## 6.371193e+12 : -1.922326e+00 -4.855256e-01 -5.789681e-01 -4.405781e-04 4.048477e-04 -1.132038e-09
## 1.590227e+12 : -3.385858e+00 -1.294959e-01 -2.899297e-01 -2.187966e-04 4.037949e-04 -2.100189e-09
## 19889209 : -4.850624e+00 2.266128e-01 -8.927502e-04 3.128700e-06 3.991144e-04 -5.877643e-09 2.6
## 825292.5 : -4.854099e+00 2.244501e-01 -7.872443e-04 1.327192e-06 8.773391e-04 4.504172e-08 -1.1
## 72834.96 : -4.698904e+00 2.158071e-01 -6.255161e-04 8.206990e-07 1.206312e-03 1.711327e-06 -1.2
## 11897.69 : -4.260919e+00 1.962288e-01 -4.518142e-04 6.174559e-07 5.394675e-04 9.144746e-06 -6.2
## 3068.102 : -3.363680e+00 1.545785e-01 -1.051538e-04 4.250646e-07 -1.433242e-03 2.984461e-05 -2.0
```

```
## 909.5887 : -1.947093e+00  8.097392e-02  6.980495e-04 -2.856405e-08 -4.239912e-03  7.556907e-05 -5.3
## 220.8618 : -4.057550e-01 -1.376339e-02  2.096694e-03 -9.279485e-07 -6.080614e-03  1.470438e-04 -1.0
## 31.88262 :  7.090768e-01 -9.381732e-02  3.536101e-03 -1.838264e-06 -6.162496e-03  2.145881e-04 -1.4
## 3.200182 :  1.102048e+00 -1.249213e-01  4.149347e-03 -1.951524e-06 -5.756966e-03  2.422411e-04 -1.4
## 1.55733 :  1.100520e+00 -1.246480e-01  4.131519e-03 -1.571143e-06 -5.729023e-03  2.422069e-04 -1.30
## 1.532465 :  1.080053e+00 -1.228904e-01  4.090638e-03 -1.435504e-06 -5.758189e-03  2.407076e-04 -1.2
## 1.532438 :  1.077745e+00 -1.227015e-01  4.086549e-03 -1.426532e-06 -5.760914e-03  2.405448e-04 -1.2
## 1.532438 :  1.077639e+00 -1.226932e-01  4.086381e-03 -1.426274e-06 -5.760992e-03  2.405376e-04 -1.2
```

```
summary(mcc_Cu)
```

```
##
## Formula: Cu_CTE ~ ((a0 + a1 * temp_K + a2 * temp_K^2 + a3 * temp_K^3)/(1 +
##      b1 * temp_K + b2 * temp_K^2 + b3 * temp_K^3))
##
## Parameters:
##      Estimate Std. Error t value Pr(>|t|)
## a0  1.078e+00  1.707e-01   6.313 1.40e-09 ***
## a1 -1.227e-01  1.200e-02 -10.224 < 2e-16 ***
## a2  4.086e-03  2.251e-04  18.155 < 2e-16 ***
## a3 -1.426e-06  2.758e-07  -5.172 5.06e-07 ***
## b1 -5.761e-03  2.471e-04 -23.312 < 2e-16 ***
## b2  2.405e-04  1.045e-05  23.019 < 2e-16 ***
## b3 -1.231e-07  1.303e-08  -9.453 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.0818 on 229 degrees of freedom
##
## Number of iterations to convergence: 23
## Achieved convergence tolerance: 1.664e-06
```

```
glance(mcc_Cu)
```

```
##      sigma isConv      finTol  logLik      AIC      BIC deviance
## 1 0.08180385  TRUE 1.664197e-06 259.4932 -502.9863 -475.2757 1.532438
## df.residual
## 1      229
```

```
augment(mcc_Cu)
```

```
##      temp_K Cu_CTE      .fitted      .resid
## 1    24.41  0.591  0.4963639  0.094636113
## 2    34.82  1.547  1.5653400 -0.018340010
## 3    44.09  2.902  2.9005739  0.001426132
## 4    45.07  2.894  3.0533083 -0.159308281
## 5    54.98  4.703  4.6386624  0.064337570
## 6    65.51  6.307  6.2804623  0.026537706
## 7    70.53  7.030  7.0126772  0.017322841
## 8    75.70  7.898  7.7231356  0.174864443
## 9    89.57  9.470  9.3955397  0.074460287
## 10   91.14  9.484  9.5636985 -0.079698527
## 11   96.40 10.072 10.0975170 -0.025516971
## 12   97.19 10.163 10.1738762 -0.010876165
## 13  114.26 11.615 11.6058598  0.009140235
## 14  120.25 12.005 12.0216811 -0.016681059
```

```
## 15 127.08 12.478 12.4499677 0.028032300
## 16 133.55 12.982 12.8157611 0.166238889
## 17 133.61 12.970 12.8189865 0.151013467
## 18 158.67 13.926 13.9459607 -0.019960705
## 19 172.74 14.452 14.4277145 0.024285466
## 20 171.31 14.404 14.3826277 0.021372299
## 21 202.14 15.190 15.2041280 -0.014127993
## 22 220.55 15.550 15.5795355 -0.029535518
## 23 221.05 15.528 15.5888324 -0.060832403
## 24 221.39 15.499 15.5951299 -0.096129866
## 25 250.99 16.131 16.0783145 0.052685472
## 26 268.99 16.438 16.3224628 0.115537197
## 27 271.80 16.387 16.3579471 0.029052870
## 28 271.97 16.549 16.3600733 0.188926721
## 29 321.31 16.872 16.8979959 -0.025995876
## 30 321.69 16.830 16.9016483 -0.071648338
## 31 330.14 16.926 16.9813826 -0.055382599
## 32 333.03 16.907 17.0080323 -0.101032295
## 33 333.47 16.966 17.0120633 -0.046063327
## 34 340.77 17.060 17.0779701 -0.017970082
## 35 345.65 17.122 17.1210593 0.000940730
## 36 373.11 17.311 17.3512466 -0.040246649
## 37 373.79 17.355 17.3567171 -0.001717084
## 38 411.82 17.668 17.6493340 0.018665965
## 39 419.51 17.767 17.7059105 0.061089474
## 40 421.59 17.803 17.7210942 0.081905760
## 41 422.02 17.765 17.7242272 0.040772842
## 42 422.47 17.768 17.7275036 0.040496385
## 43 422.61 17.736 17.7285225 0.007477495
## 44 441.75 17.858 17.8659854 -0.007985381
## 45 447.41 17.877 17.9060218 -0.029021763
## 46 448.70 17.912 17.9151127 -0.003112748
## 47 472.89 18.046 18.0836406 -0.037640604
## 48 476.69 18.085 18.1098368 -0.024836835
## 49 522.47 18.291 18.4221886 -0.131188615
## 50 522.62 18.357 18.4232070 -0.066206966
## 51 524.43 18.426 18.4354946 -0.009494602
## 52 546.75 18.584 18.5870962 -0.003096202
## 53 549.53 18.610 18.6060088 0.003991184
## 54 575.29 18.870 18.7819540 0.088045977
## 55 576.00 18.795 18.7868265 0.008173532
## 56 625.55 19.111 19.1315632 -0.020563155
## 57 20.15 0.367 0.2578734 0.109126633
## 58 28.78 0.796 0.8706755 -0.074675533
## 59 29.57 0.892 0.9508152 -0.058815215
## 60 37.41 1.903 1.9126172 -0.009617204
## 61 39.12 2.150 2.1545245 -0.004524486
## 62 50.24 3.697 3.8760413 -0.179041267
## 63 61.38 5.870 5.6506367 0.219363250
## 64 66.25 6.421 6.3908398 0.030160222
## 65 73.42 7.422 7.4155213 0.006478695
## 66 95.52 9.944 10.0113074 -0.067307437
## 67 107.32 11.023 11.0710890 -0.048089021
## 68 122.04 11.870 12.1384228 -0.268422792
```

```
## 69 134.03 12.786 12.8414824 -0.055482433
## 70 163.19 14.067 14.1104537 -0.043453696
## 71 163.48 13.974 14.1206749 -0.146674921
## 72 175.70 14.462 14.5185343 -0.056534286
## 73 179.86 14.464 14.6407452 -0.176745156
## 74 211.27 15.381 15.3987890 -0.017789027
## 75 217.78 15.483 15.5272412 -0.044241243
## 76 219.14 15.590 15.5530853 0.036914739
## 77 262.52 16.075 16.2382086 -0.163208614
## 78 268.01 16.347 16.3099337 0.037066300
## 79 268.62 16.181 16.3177419 -0.136741912
## 80 336.25 16.915 17.0373752 -0.122375209
## 81 337.23 17.003 17.0462347 -0.043234658
## 82 339.33 16.978 17.0651106 -0.087110573
## 83 427.38 17.756 17.7631127 -0.007112672
## 84 428.58 17.808 17.7717775 0.036222457
## 85 432.68 17.868 17.8012757 0.066724340
## 86 528.99 18.481 18.4664497 0.014550340
## 87 531.08 18.486 18.4806380 0.005362040
## 88 628.34 19.090 19.1513119 -0.061311930
## 89 253.24 16.062 16.1105736 -0.048573567
## 90 273.13 16.337 16.3745196 -0.037519609
## 91 273.66 16.345 16.3810847 -0.036084688
## 92 282.10 16.388 16.4827743 -0.094774326
## 93 346.62 17.159 17.1295367 0.029463321
## 94 347.19 17.116 17.1345051 -0.018505086
## 95 348.78 17.164 17.1483135 0.015686490
## 96 351.18 17.123 17.1690174 -0.046017428
## 97 450.10 17.979 17.9249654 0.054034648
## 98 450.35 17.974 17.9267233 0.047276717
## 99 451.92 18.007 17.9377531 0.069246851
## 100 455.56 17.993 17.9632617 0.029738317
## 101 552.22 18.523 18.6243198 -0.101319806
## 102 553.56 18.669 18.6334455 0.035554457
## 103 555.74 18.617 18.6482984 -0.031298442
## 104 652.59 19.371 19.3248625 0.046137474
## 105 656.20 19.330 19.3510119 -0.021011943
## 106 14.13 0.080 0.1612725 -0.081272481
## 107 20.41 0.248 0.2685479 -0.020547945
## 108 31.30 1.089 1.1383031 -0.049303084
## 109 33.84 1.418 1.4408211 -0.022821106
## 110 39.70 2.278 2.2385532 0.039446784
## 111 48.83 3.624 3.6497122 -0.025712192
## 112 54.50 4.574 4.5616267 0.012373331
## 113 60.41 5.556 5.4996610 0.056338998
## 114 72.77 7.267 7.3261617 -0.059161721
## 115 75.25 7.695 7.6631465 0.031853502
## 116 86.84 9.136 9.0931449 0.042855052
## 117 94.88 9.959 9.9478398 0.011160239
## 118 96.40 9.957 10.0975170 -0.140516971
## 119 117.37 11.600 11.8267293 -0.226729304
## 120 139.08 13.138 13.1011146 0.036885374
## 121 147.73 13.564 13.5032486 0.060751378
## 122 158.63 13.871 13.9444602 -0.073460197
```

```
## 123 161.84 13.994 14.0623548 -0.068354756
## 124 192.11 14.947 14.9677463 -0.020746271
## 125 206.76 15.473 15.3048785 0.168121477
## 126 209.07 15.379 15.3535064 0.025493579
## 127 213.32 15.455 15.4401119 0.014888101
## 128 226.44 15.908 15.6864092 0.221590783
## 129 237.12 16.114 15.8666313 0.247368679
## 130 330.90 17.071 16.9884203 0.082579731
## 131 358.72 17.135 17.2330261 -0.098026092
## 132 370.77 17.282 17.3323460 -0.050345962
## 133 372.72 17.368 17.3481047 0.019895254
## 134 396.24 17.483 17.5323108 -0.049310842
## 135 416.59 17.764 17.6845113 0.079488723
## 136 484.02 18.185 18.1602046 0.024795393
## 137 495.47 18.271 18.2385282 0.032471776
## 138 514.78 18.236 18.3699663 -0.133966278
## 139 515.65 18.237 18.3758764 -0.138876358
## 140 519.47 18.523 18.4018198 0.121180208
## 141 544.47 18.627 18.5715926 0.055407414
## 142 560.11 18.665 18.6780990 -0.013099005
## 143 620.77 19.086 19.0978246 -0.011824627
## 144 18.97 0.214 0.2160310 -0.002031040
## 145 28.93 0.943 0.8856173 0.057382657
## 146 33.91 1.429 1.4495793 -0.020579292
## 147 40.03 2.241 2.2867741 -0.045774104
## 148 44.66 2.951 2.9892364 -0.038236434
## 149 49.87 3.782 3.8165695 -0.034569455
## 150 55.16 4.757 4.6675252 0.089474794
## 151 60.90 5.602 5.5760576 0.025942404
## 152 72.08 7.169 7.2305064 -0.061506448
## 153 85.15 8.920 8.8994792 0.020520834
## 154 97.06 10.055 10.1613775 -0.106377474
## 155 119.63 12.035 11.9804653 0.054534701
## 156 133.27 12.861 12.8006702 0.060329793
## 157 143.84 13.436 13.3286469 0.107353146
## 158 161.91 14.167 14.0648699 0.102130081
## 159 180.67 14.755 14.6638377 0.091162293
## 160 198.44 15.168 15.1198750 0.048125043
## 161 226.86 15.651 15.6938160 -0.042816044
## 162 229.65 15.746 15.7423289 0.003671052
## 163 258.27 16.216 16.1807994 0.035200620
## 164 273.77 16.445 16.3824445 0.062555507
## 165 339.15 16.965 17.0634984 -0.098498370
## 166 350.13 17.121 17.1599798 -0.038979782
## 167 362.75 17.206 17.2666301 -0.060630075
## 168 371.03 17.250 17.3344519 -0.084451920
## 169 393.32 17.339 17.5099757 -0.170975691
## 170 448.53 17.793 17.9139154 -0.120915404
## 171 473.78 18.123 18.0897817 0.033218343
## 172 511.12 18.490 18.3450954 0.144904609
## 173 524.70 18.566 18.4373275 0.128672496
## 174 548.75 18.645 18.6007013 0.044298675
## 175 551.64 18.706 18.6203708 0.085629235
## 176 574.02 18.924 18.7732422 0.150757834
```

```
## 177 623.86 19.100 19.1196210 -0.019620959
## 178 21.46 0.375 0.3169130 0.058086952
## 179 24.33 0.471 0.4906796 -0.019679635
## 180 33.43 1.504 1.3899566 0.114043426
## 181 39.22 2.204 2.1689447 0.035055321
## 182 44.18 2.813 2.9145398 -0.101539787
## 183 55.02 4.765 4.6450777 0.119922345
## 184 94.33 9.835 9.8927746 -0.057774647
## 185 96.44 10.040 10.1014067 -0.061406663
## 186 118.82 11.946 11.9260020 0.019998000
## 187 128.48 12.596 12.5322413 0.063758682
## 188 141.94 13.303 13.2397256 0.063274444
## 189 156.92 13.922 13.8795489 0.042451100
## 190 171.65 14.440 14.3934209 0.046579088
## 191 190.00 14.951 14.9146360 0.036363980
## 192 223.26 15.627 15.6294176 -0.002417573
## 193 223.88 15.639 15.6406575 -0.001657497
## 194 231.50 15.814 15.7738532 0.040146846
## 195 265.05 16.315 16.2715923 0.043407743
## 196 269.44 16.334 16.3281890 0.005810976
## 197 271.78 16.430 16.3576968 0.072303157
## 198 273.46 16.423 16.3786099 0.044390110
## 199 334.61 17.024 17.0224756 0.001524429
## 200 339.79 17.009 17.0692258 -0.060225818
## 201 349.52 17.165 17.1547149 0.010285129
## 202 358.18 17.134 17.2284921 -0.094492125
## 203 377.98 17.349 17.3902120 -0.041211980
## 204 394.77 17.576 17.5210839 0.054916093
## 205 429.66 17.848 17.7795636 0.068436368
## 206 468.22 18.090 18.0513573 0.038642735
## 207 487.27 18.276 18.1824758 0.093524152
## 208 519.54 18.404 18.4022951 0.001704889
## 209 523.03 18.519 18.4259904 0.093009575
## 210 612.99 19.133 19.0431600 0.089840025
## 211 638.59 19.074 19.2242391 -0.150239081
## 212 641.36 19.239 19.2440522 -0.005052151
## 213 622.05 19.280 19.1068475 0.173152498
## 214 631.50 19.101 19.1737313 -0.072731259
## 215 663.97 19.398 19.4075930 -0.009592967
## 216 646.90 19.252 19.2838185 -0.031818479
## 217 748.29 19.890 20.0529391 -0.162939136
## 218 749.21 20.007 20.0603469 -0.053346895
## 219 750.14 19.929 20.0678442 -0.138844239
## 220 647.04 19.268 19.2848259 -0.016825875
## 221 646.89 19.324 19.2837465 0.040253473
## 222 746.90 20.049 20.0417638 0.007236178
## 223 748.43 20.107 20.0540658 0.052934170
## 224 747.35 20.062 20.0453795 0.016620484
## 225 749.27 20.065 20.0608303 0.004169680
## 226 647.61 19.286 19.2889287 -0.002928687
## 227 747.78 19.972 20.0488365 -0.076836491
## 228 750.51 20.088 20.0708296 0.017170406
## 229 851.37 20.743 20.9461745 -0.203174508
## 230 845.97 20.830 20.8958249 -0.065824945
```

```
## 231 847.54 20.935 20.9104183 0.024581707
## 232 849.93 21.035 20.9327049 0.102295138
## 233 851.61 20.930 20.9484225 -0.018422516
## 234 849.75 21.074 20.9310234 0.142976630
## 235 850.98 21.085 20.9425234 0.142476633
## 236 848.23 20.935 20.9168436 0.018156359
```

```
tidy(mcc_Cu)
```

```
##   term      estimate  std.error statistic    p.value
## 1  a0  1.077639e+00 1.707017e-01   6.312994 1.404129e-09
## 2  a1 -1.226932e-01 1.200030e-02 -10.224180 1.866827e-20
## 3  a2  4.086381e-03 2.250834e-04  18.154961 3.109432e-46
## 4  a3 -1.426274e-06 2.757806e-07  -5.171771 5.055842e-07
## 5  b1 -5.760992e-03 2.471290e-04 -23.311682 2.178299e-62
## 6  b2  2.405376e-04 1.044939e-05  23.019305 1.657786e-61
## 7  b3 -1.231449e-07 1.302735e-08  -9.452798 4.078186e-18
```

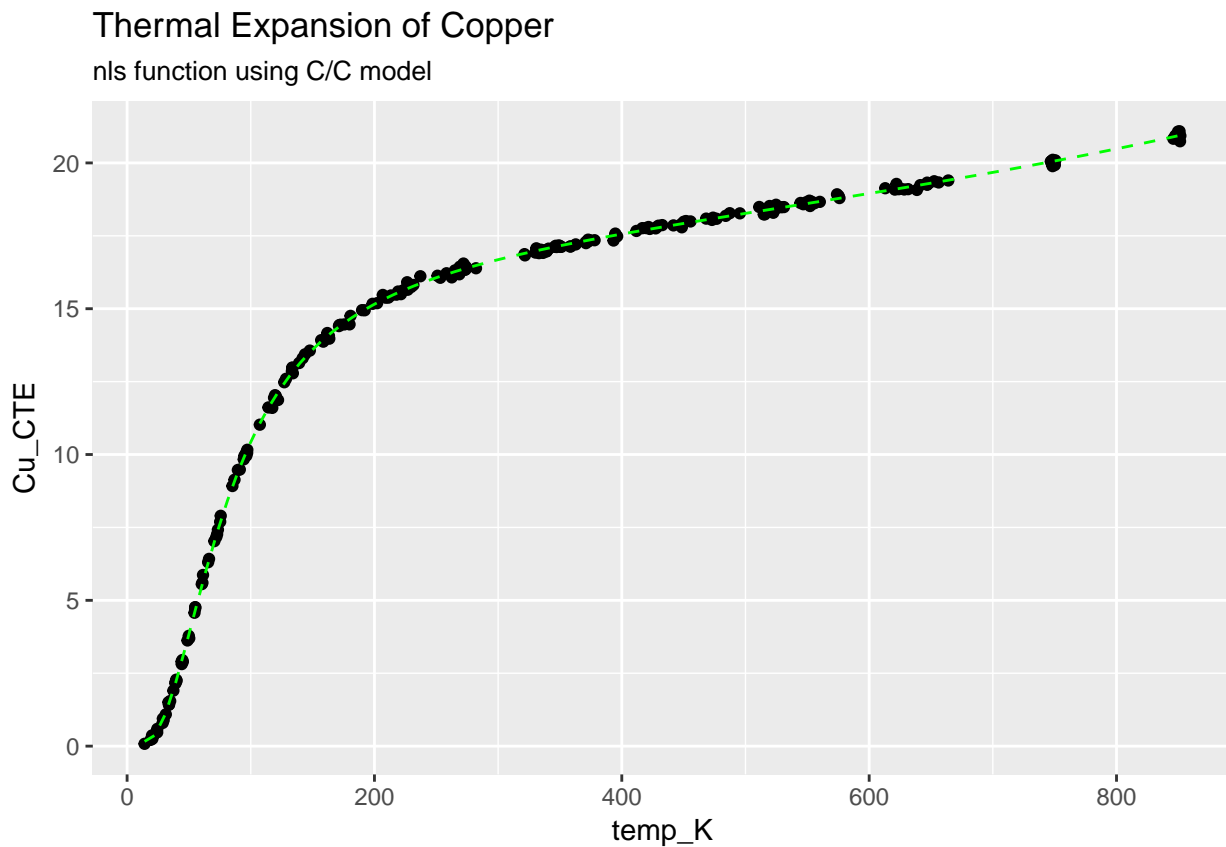
#### 4.3.4.1 Create a function using the fit parameters

```
cc.Cu.fit <- function(x) {
  ((summary(mcc_Cu)$coefficients[1] + summary(mcc_Cu)$coefficients[2]*x +
    summary(mcc_Cu)$coefficients[3]*x^2 + summary(mcc_Cu)$coefficients[4]*x^3)/(1 + summary(mcc_Cu)$c
```

#### 4.3.4.2 Add the fitted curve to the graph

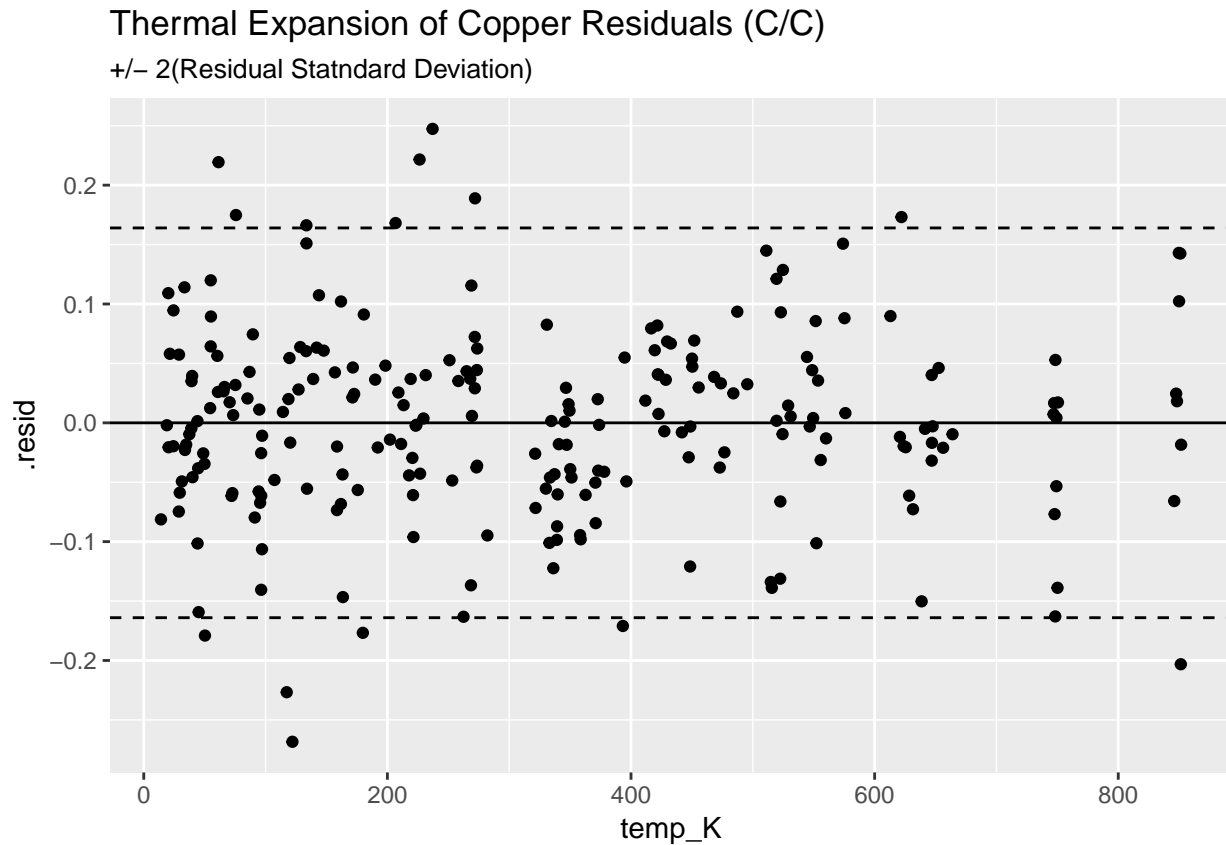
```
ggplot(CTECu, aes(temp_K, Cu_CTE)) +
  geom_point() +
  stat_function(fun = cc.Cu.fit, colour = "green", linetype = "dashed") +
  ggtitle("Thermal Expansion of Copper", subtitle = "nls function using C/C model")
```





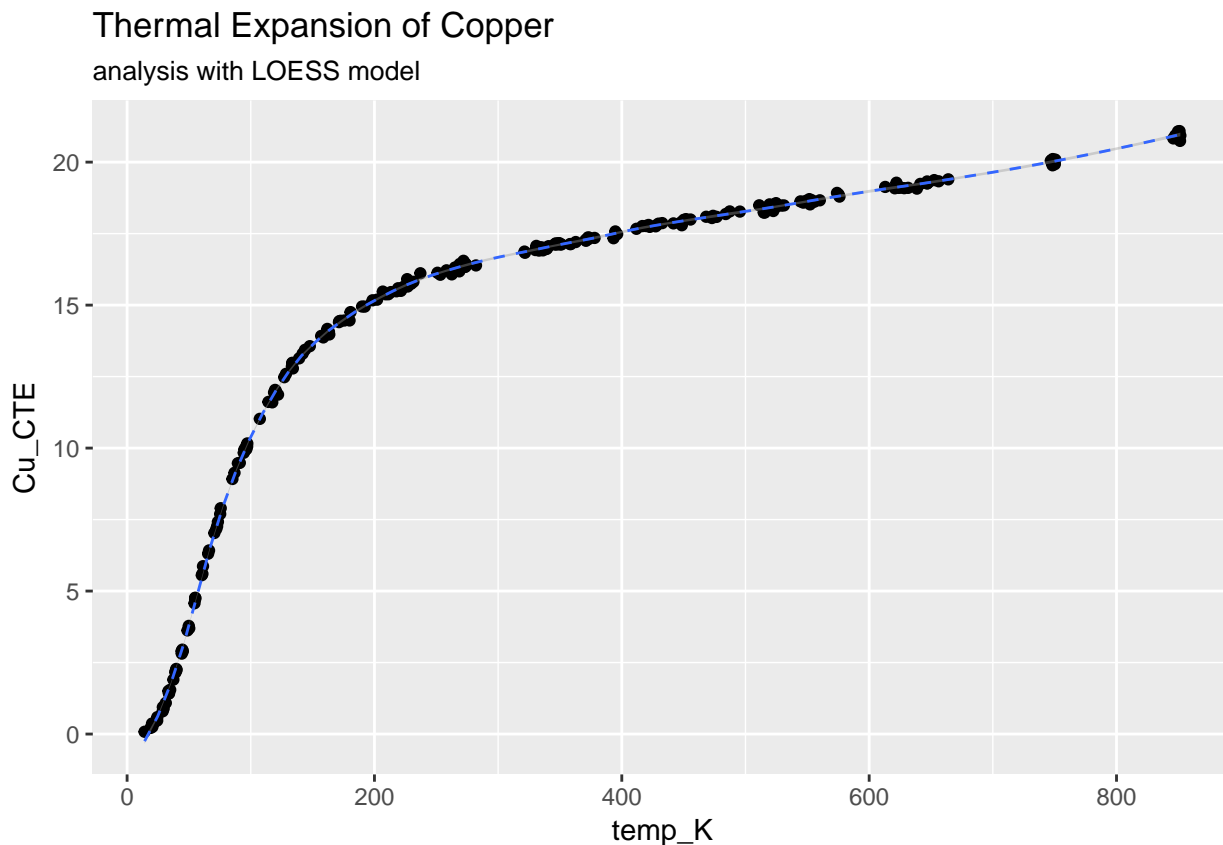
#### 4.3.4.3 Plot the residuals from the C/C model

```
ggplot(augment(mcc_Cu)) +
  geom_point(aes(temp_K, .resid)) +
  geom_hline(aes(yintercept=0)) +
  geom_hline(aes(yintercept=+2*0.082), linetype = "dashed") +
  geom_hline(aes(yintercept=-2*0.082), linetype = "dashed") +
  ggtitle("Thermal Expansion of Copper Residuals (C/C)", subtitle = "+/- 2(Residual Standard Deviation)")
```



4.3.4.4 Finally, lets fit the data with th LOESS method and compare to the C/C model

```
ggplot(CTECu, aes(temp_K, Cu_CTE)) +
  geom_point() +
  stat_smooth(method = "loess", span = 0.2, linetype = "dashed", size = 0.5) +
  ggtitle("Thermal Expansion of Copper", subtitle = "analysis with LOESS model")
```



We can look at the quality of the fit using the LOESS model directly

```
mloess_Cu <- loess(Cu_CTE ~ temp_K, CTECu, span = 0.2)
```

```
summary(mloess_Cu)
```

```
## Call:
## loess(formula = Cu_CTE ~ temp_K, data = CTECu, span = 0.2)
##
## Number of Observations: 236
## Equivalent Number of Parameters: 15.02
## Residual Standard Error: 0.09039
## Trace of smoother matrix: 16.62 (exact)
##
## Control settings:
##   span      : 0.2
##   degree    : 2
##   family    : gaussian
##   surface   : interpolate      cell = 0.2
##   normalize : TRUE
##   parametric: FALSE
##   drop.square: FALSE
```

```
augment(mloess_Cu)
```

```
##   Cu_CTE temp_K   .fitted   .se.fit   .resid
## 1    0.591  24.41  0.5893886 0.02340924 1.611396e-03
## 2    1.547  34.82  1.7035504 0.01790375 -1.565504e-01
```

```

## 3    2.902  44.09  2.9075529 0.01956124 -5.552921e-03
## 4    2.894  45.07  3.0426764 0.01971197 -1.486764e-01
## 5    4.703  54.98  4.6006680 0.02177693  1.023320e-01
## 6    6.307  65.51  6.2727258 0.02223313  3.427422e-02
## 7    7.030  70.53  7.0291230 0.02424350  8.770125e-04
## 8    7.898  75.70  7.7223713 0.02316620  1.756287e-01
## 9    9.470  89.57  9.3678543 0.02312016  1.021457e-01
## 10   9.484  91.14  9.5326204 0.02293994 -4.862038e-02
## 11  10.072  96.40 10.0532384 0.02243139  1.876162e-02
## 12  10.163  97.19 10.1306239 0.02241359  3.237612e-02
## 13  11.615 114.26 11.5706405 0.02163989  4.435953e-02
## 14  12.005 120.25 12.0049191 0.02295519  8.089826e-05
## 15  12.478 127.08 12.4554822 0.02242131  2.251778e-02
## 16  12.982 133.55 12.8408206 0.02259261  1.411794e-01
## 17  12.970 133.61 12.8442640 0.02259171  1.257360e-01
## 18  13.926 158.67 13.9557957 0.02266600 -2.979572e-02
## 19  14.452 172.74 14.4192091 0.02364575  3.279085e-02
## 20  14.404 171.31 14.3758966 0.02330013  2.810341e-02
## 21  15.190 202.14 15.2087537 0.02229812 -1.875374e-02
## 22  15.550 220.55 15.6042108 0.02178006 -5.421077e-02
## 23  15.528 221.05 15.6140038 0.02182985 -8.600384e-02
## 24  15.499 221.39 15.6206473 0.02185661 -1.216473e-01
## 25  16.131 250.99 16.1091714 0.01914307  2.182861e-02
## 26  16.438 268.99 16.3398608 0.02202205  9.813921e-02
## 27  16.387 271.80 16.3734167 0.02243304  1.358326e-02
## 28  16.549 271.97 16.3754236 0.02245998  1.735764e-01
## 29  16.872 321.31 16.8639118 0.02213125  8.088198e-03
## 30  16.830 321.69 16.8672482 0.02215705 -3.724821e-02
## 31  16.926 330.14 16.9420265 0.02190354 -1.602647e-02
## 32  16.907 333.03 16.9680613 0.02136006 -6.106125e-02
## 33  16.966 333.47 16.9720533 0.02124855 -6.053335e-03
## 34  17.060 340.77 17.0380252 0.01915004  2.197485e-02
## 35  17.122 345.65 17.0800345 0.01826731  4.196548e-02
## 36  17.311 373.11 17.3095335 0.02446425  1.466498e-03
## 37  17.355 373.79 17.3154949 0.02456639  3.950514e-02
## 38  17.668 411.82 17.6648664 0.02216767  3.133620e-03
## 39  17.767 419.51 17.7287099 0.02243940  3.829015e-02
## 40  17.803 421.59 17.7448828 0.02218004  5.811720e-02
## 41  17.765 422.02 17.7481608 0.02211155  1.683925e-02
## 42  17.768 422.47 17.7515723 0.02203853  1.642772e-02
## 43  17.736 422.61 17.7526301 0.02201581 -1.663008e-02
## 44  17.858 441.75 17.8917493 0.02046968 -3.374927e-02
## 45  17.877 447.41 17.9304245 0.02154521 -5.342452e-02
## 46  17.912 448.70 17.9393108 0.02179951 -2.731083e-02
## 47  18.046 472.89 18.0999205 0.02478693 -5.392046e-02
## 48  18.085 476.69 18.1246418 0.02573444 -3.964181e-02
## 49  18.291 522.47 18.4283764 0.02104353 -1.373764e-01
## 50  18.357 522.62 18.4294420 0.02102223 -7.244200e-02
## 51  18.426 524.43 18.4423209 0.02071864 -1.632094e-02
## 52  18.584 546.75 18.6034919 0.02059169 -1.949187e-02
## 53  18.610 549.53 18.6244942 0.02087707 -1.449418e-02
## 54  18.870 575.29 18.8101404 0.02332466  5.985959e-02
## 55  18.795 576.00 18.8151025 0.02335059 -2.010248e-02
## 56  19.111 625.55 19.1441090 0.02323769 -3.310901e-02

```

```

## 57  0.367  20.15  0.2116990 0.03085448  1.553010e-01
## 58  0.796  28.78  1.0242942 0.01913119 -2.282942e-01
## 59  0.892  29.57  1.1083269 0.01870637 -2.163269e-01
## 60  1.903  37.41  2.0202956 0.01828370 -1.172956e-01
## 61  2.150  39.12  2.2397801 0.01860451 -8.978013e-02
## 62  3.697  50.24  3.8425643 0.02049747 -1.455643e-01
## 63  5.870  61.38  5.6119898 0.02116325  2.580102e-01
## 64  6.421  66.25  6.3886426 0.02256694  3.235736e-02
## 65  7.422  73.42  7.4232996 0.02409276 -1.299626e-03
## 66  9.944  95.52  9.9668213 0.02241709 -2.282127e-02
## 67 11.023 107.32 11.0307166 0.02035314 -7.716646e-03
## 68 11.870 122.04 12.1285181 0.02287899 -2.585181e-01
## 69 12.786 134.03 12.8683172 0.02258018 -8.231716e-02
## 70 14.067 163.19 14.1199802 0.02247130 -5.298022e-02
## 71 13.974 163.48 14.1297883 0.02245355 -1.557883e-01
## 72 14.462 175.70 14.5100999 0.02412487 -4.809988e-02
## 73 14.464 179.86 14.6359457 0.02384732 -1.719457e-01
## 74 15.381 211.27 15.4148497 0.02158281 -3.384974e-02
## 75 15.483 217.78 15.5493643 0.02140571 -6.636426e-02
## 76 15.590 219.14 15.5764283 0.02159609  1.357166e-02
## 77 16.075 262.52 16.2591976 0.02071960 -1.841976e-01
## 78 16.347 268.01 16.3276907 0.02191144  1.930926e-02
## 79 16.181 268.62 16.3352840 0.02198209 -1.542840e-01
## 80 16.915 336.25 16.9973389 0.02032597 -8.233893e-02
## 81 17.003 337.23 17.0062403 0.02000511 -3.240328e-03
## 82 16.978 339.33 17.0252000 0.01945679 -4.719998e-02
## 83 17.756 427.38 17.7882079 0.02146238 -3.220789e-02
## 84 17.808 428.58 17.7972085 0.02139069  1.079149e-02
## 85 17.868 432.68 17.8279861 0.02096926  4.001391e-02
## 86 18.481 528.99 18.4749238 0.01983701  6.076167e-03
## 87 18.486 531.08 18.4899317 0.01953248 -3.931729e-03
## 88 19.090 628.34 19.1609875 0.02259820 -7.098748e-02
## 89 16.062 253.24 16.1395756 0.01902599 -7.757559e-02
## 90 16.337 273.13 16.3892160 0.02262455 -5.221599e-02
## 91 16.345 273.66 16.3956097 0.02268052 -5.060973e-02
## 92 16.388 282.10 16.4926643 0.02260402 -1.046643e-01
## 93 17.159 346.62 17.0882502 0.01830996  7.074984e-02
## 94 17.116 347.19 17.0930759 0.01837768  2.292413e-02
## 95 17.164 348.78 17.1065650 0.01870251  5.743503e-02
## 96 17.123 351.18 17.1271492 0.01934207 -4.149195e-03
## 97 17.979 450.10 17.9490269 0.02201781  2.997309e-02
## 98 17.974 450.35 17.9507714 0.02204810  2.322857e-02
## 99 18.007 451.92 17.9616731 0.02219872  4.532692e-02
## 100 17.993 455.56 17.9865023 0.02238314  6.497679e-03
## 101 18.523 552.22 18.6450517 0.02125465 -1.220517e-01
## 102 18.669 553.56 18.6552772 0.02147989  1.372284e-02
## 103 18.617 555.74 18.6717598 0.02187462 -5.475980e-02
## 104 19.371 652.59 19.3156329 0.02348120  5.536710e-02
## 105 19.330 656.20 19.3403259 0.02347526 -1.032591e-02
## 106  0.080  14.13 -0.2493998 0.04620251  3.293998e-01
## 107  0.248  20.41  0.2334920 0.03031239  1.450797e-02
## 108  1.089  31.30  1.2980967 0.01809055 -2.090967e-01
## 109  1.418  33.84  1.5885439 0.01783812 -1.705439e-01
## 110  2.278  39.70  2.3157401 0.01871910 -3.774011e-02

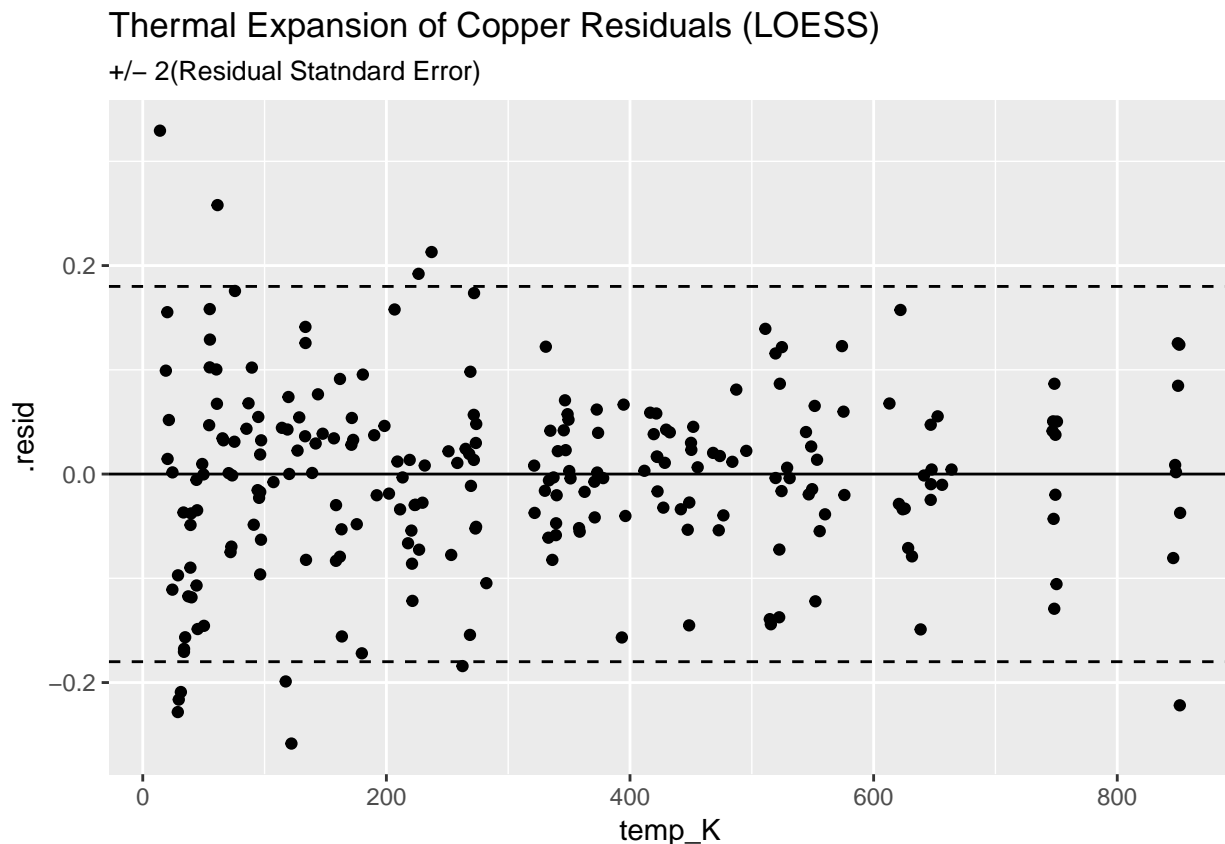
```

```
## 111 3.624 48.83 3.6143394 0.02014915 9.660635e-03
## 112 4.574 54.50 4.5271268 0.02174540 4.687324e-02
## 113 5.556 60.41 5.4556488 0.02116604 1.003512e-01
## 114 7.267 72.77 7.3366019 0.02425223 -6.960186e-02
## 115 7.695 75.25 7.6639677 0.02337864 3.103232e-02
## 116 9.136 86.84 9.0681217 0.02259302 6.787825e-02
## 117 9.959 94.88 9.9042264 0.02241509 5.477360e-02
## 118 9.957 96.40 10.0532384 0.02243139 -9.623838e-02
## 119 11.600 117.37 11.7989267 0.02256946 -1.989267e-01
## 120 13.138 139.08 13.1369635 0.02161945 1.036507e-03
## 121 13.564 147.73 13.5252987 0.02034951 3.870126e-02
## 122 13.871 158.63 13.9542333 0.02266416 -8.323330e-02
## 123 13.994 161.84 14.0732954 0.02256812 -7.929537e-02
## 124 14.947 192.11 14.9673282 0.02138477 -2.032820e-02
## 125 15.473 206.76 15.3151149 0.02240447 1.578851e-01
## 126 15.379 209.07 15.3669923 0.02203888 1.200768e-02
## 127 15.455 213.32 15.4582440 0.02127550 -3.244012e-03
## 128 15.908 226.44 15.7159178 0.02202286 1.920822e-01
## 129 16.114 237.12 15.9010123 0.02219862 2.129877e-01
## 130 17.071 330.90 16.9488424 0.02178562 1.221576e-01
## 131 17.135 358.72 17.1902627 0.02080437 -5.526271e-02
## 132 17.282 370.77 17.2893556 0.02397387 -7.355555e-03
## 133 17.368 372.72 17.3061323 0.02439585 6.186773e-02
## 134 17.483 396.24 17.5232072 0.02129821 -4.020717e-02
## 135 17.764 416.59 17.7051251 0.02251976 5.887493e-02
## 136 18.185 484.02 18.1732409 0.02658515 1.175908e-02
## 137 18.271 495.47 18.2487424 0.02413964 2.225757e-02
## 138 18.236 514.78 18.3751895 0.02146154 -1.391895e-01
## 139 18.237 515.65 18.3810788 0.02145767 -1.440788e-01
## 140 18.523 519.47 18.4073027 0.02134191 1.156973e-01
## 141 18.627 544.47 18.5866978 0.02039557 4.030219e-02
## 142 18.665 560.11 18.7036081 0.02255376 -3.860805e-02
## 143 19.086 620.77 19.1146279 0.02451487 -2.862791e-02
## 144 0.214 18.97 0.1147946 0.03344855 9.920537e-02
## 145 0.943 28.93 1.0401129 0.01904309 -9.711289e-02
## 146 1.429 33.91 1.5967118 0.01784020 -1.677118e-01
## 147 2.241 40.03 2.3592580 0.01878496 -1.182580e-01
## 148 2.951 44.66 2.9857198 0.01965356 -3.471981e-02
## 149 3.782 49.87 3.7823568 0.02039192 -3.567609e-04
## 150 4.757 55.16 4.6280117 0.02177796 1.289883e-01
## 151 5.602 60.90 5.5345962 0.02115332 6.740384e-02
## 152 7.169 72.08 7.2438760 0.02434648 -7.487605e-02
## 153 8.920 85.15 8.8765497 0.02201842 4.345026e-02
## 154 10.055 97.06 10.1179699 0.02242059 -6.296988e-02
## 155 12.035 119.63 11.9610696 0.02293092 7.393042e-02
## 156 12.861 133.27 12.8247261 0.02259458 3.627390e-02
## 157 13.436 143.84 13.3595004 0.02046845 7.649958e-02
## 158 14.167 161.91 14.0757601 0.02256296 9.123987e-02
## 159 14.755 180.67 14.6595578 0.02369360 9.544219e-02
## 160 15.168 198.44 15.1218205 0.02179637 4.617947e-02
## 161 15.651 226.86 15.7235686 0.02203213 -7.256862e-02
## 162 15.746 229.65 15.7734814 0.02211877 -2.748143e-02
## 163 16.216 258.27 16.2053310 0.01963096 1.066899e-02
## 164 16.445 273.77 16.3969366 0.02269081 4.806339e-02
```

```
## 165 16.965 339.15 17.0235835 0.01949557 -5.858347e-02
## 166 17.121 350.13 17.1180966 0.01906644 2.903356e-03
## 167 17.206 362.75 17.2230444 0.02170905 -1.704439e-02
## 168 17.250 371.03 17.2915718 0.02403694 -4.157182e-02
## 169 17.339 393.32 17.4957437 0.02172636 -1.567437e-01
## 170 17.793 448.53 17.9381365 0.02176832 -1.451365e-01
## 171 18.123 473.78 18.1056936 0.02501800 1.730638e-02
## 172 18.490 511.12 18.3506976 0.02148107 1.393024e-01
## 173 18.566 524.70 18.4442453 0.02066771 1.217547e-01
## 174 18.645 548.75 18.6185616 0.02078771 2.643841e-02
## 175 18.706 551.64 18.6406162 0.02116414 6.538383e-02
## 176 18.924 574.02 18.8012573 0.02328181 1.227427e-01
## 177 19.100 623.86 19.1337700 0.02369936 -3.377002e-02
## 178 0.375 21.46 0.3231433 0.02823514 5.185672e-02
## 179 0.471 24.33 0.5818836 0.02351969 -1.108836e-01
## 180 1.504 33.43 1.5408606 0.01783466 -3.686060e-02
## 181 2.204 39.22 2.2528267 0.01862413 -4.882670e-02
## 182 2.813 44.18 2.9198854 0.01957625 -1.068854e-01
## 183 4.765 55.02 4.6067413 0.02177754 1.582587e-01
## 184 9.835 94.33 9.8504461 0.02243031 -1.544608e-02
## 185 10.040 96.44 10.0571828 0.02243189 -1.718276e-02
## 186 11.946 118.82 11.9032635 0.02284777 4.273650e-02
## 187 12.596 128.48 12.5416275 0.02240950 5.437255e-02
## 188 13.303 141.94 13.2736796 0.02084791 2.932044e-02
## 189 13.922 156.92 13.8877209 0.02247490 3.427913e-02
## 190 14.440 171.65 14.3861863 0.02338380 5.381374e-02
## 191 14.951 190.00 14.9137132 0.02157548 3.728681e-02
## 192 15.627 223.26 15.6566755 0.02194939 -2.967552e-02
## 193 15.639 223.88 15.6684179 0.02196806 -2.941790e-02
## 194 15.814 231.50 15.8057944 0.02219606 8.205561e-03
## 195 16.315 265.05 16.2908371 0.02136428 2.416293e-02
## 196 16.334 269.44 16.3453544 0.02207639 -1.135442e-02
## 197 16.430 271.78 16.3731807 0.02242985 5.681925e-02
## 198 16.423 273.46 16.3931927 0.02266094 2.980726e-02
## 199 17.024 334.61 16.9824164 0.02089562 4.158361e-02
## 200 17.009 339.79 17.0293219 0.01936440 -2.032188e-02
## 201 17.165 349.52 17.1128736 0.01889826 5.212642e-02
## 202 17.134 358.18 17.1858476 0.02070164 -5.184756e-02
## 203 17.349 377.98 17.3528982 0.02471271 -3.898163e-03
## 204 17.576 394.77 17.5093938 0.02148845 6.660620e-02
## 205 17.848 429.66 17.8054024 0.02132226 4.259762e-02
## 206 18.090 468.22 18.0696956 0.02364603 2.030442e-02
## 207 18.276 487.27 18.1949994 0.02624330 8.100057e-02
## 208 18.404 519.54 18.4077893 0.02133746 -3.789293e-03
## 209 18.519 523.03 18.4323559 0.02096056 8.664405e-02
## 210 19.133 612.99 19.0653124 0.02580219 6.768757e-02
## 211 19.074 638.59 19.2230166 0.02234591 -1.490166e-01
## 212 19.239 641.36 19.2403795 0.02270688 -1.379523e-03
## 213 19.280 622.05 19.1225896 0.02419340 1.574104e-01
## 214 19.101 631.50 19.1799682 0.02215217 -7.896818e-02
## 215 19.398 663.97 19.3936246 0.02323551 4.375380e-03
## 216 19.252 646.90 19.2767622 0.02330845 -2.476219e-02
## 217 19.890 748.29 20.0192002 0.02557545 -1.292002e-01
## 218 20.007 749.21 20.0268252 0.02554427 -1.982522e-02
```

```
## 219 19.929 750.14 20.0345476 0.02551122 -1.055476e-01
## 220 19.268 647.04 19.2777172 0.02331586 -9.717234e-03
## 221 19.324 646.89 19.2766941 0.02330790 4.730595e-02
## 222 20.049 746.90 20.0077110 0.02561713 4.128896e-02
## 223 20.107 748.43 20.0203596 0.02557081 8.664040e-02
## 224 20.062 747.35 20.0114251 0.02560513 5.057491e-02
## 225 20.065 749.27 20.0273230 0.02554218 3.767700e-02
## 226 19.286 647.61 19.2816098 0.02334364 4.390250e-03
## 227 19.972 747.78 20.0149794 0.02559209 -4.297938e-02
## 228 20.088 750.51 20.0376239 0.02549766 5.037605e-02
## 229 20.743 851.37 20.9648418 0.03249677 -2.218418e-01
## 230 20.830 845.97 20.9105761 0.03024912 -8.057613e-02
## 231 20.935 847.54 20.9262958 0.03086868 8.704217e-03
## 232 21.035 849.93 20.9503176 0.03186570 8.468244e-02
## 233 20.930 851.61 20.9672661 0.03260409 -3.726611e-02
## 234 21.074 849.75 20.9485047 0.03178839 1.254953e-01
## 235 21.085 850.98 20.9609045 0.03232366 1.240955e-01
## 236 20.935 848.23 20.9332198 0.03114992 1.780210e-03
```

```
ggplot(augment(mloess_Cu)) +
  geom_point(aes(temp_K, .resid)) +
  geom_hline(aes(yintercept=0)) +
  geom_hline(aes(yintercept=+2*(0.09)), linetype = "dashed") +
  geom_hline(aes(yintercept=-2*(0.09)), linetype = "dashed") +
  ggtitle("Thermal Expansion of Copper Residuals (LOESS)", subtitle = "+/- 2(Residual Standard Error)")
```



The C/C is slightly better, but required significantly more work.



4.3.4.5 Progaming with `case_when()`

Looking at the original data set, we can see that there are two sets of data. We might want to label these as “run1” and “run2.” we could do this in Excel using an `IF()` function. In the **tidyverse**, we can use the `case_when()` function.

```
load_cell_fit_2
```

```
##      Deflection      Load Load_squared      .fitted      .se.fit      .resid
## 1      0.11019    150000    2.2500e+10  0.1104113  8.834303e-05 -2.213214e-04
## 2      0.21956    300000    9.0000e+10  0.2200068  7.185366e-05 -4.468402e-04
## 3      0.32949    450000    2.0250e+11  0.3294601  5.888246e-05  2.987782e-05
## 4      0.43899    600000    3.6000e+11  0.4387712  4.986859e-05  2.188327e-04
## 5      0.54803    750000    5.6250e+11  0.5479400  4.495244e-05  9.002444e-05
## 6      0.65694    900000    8.1000e+11  0.6569665  4.354343e-05 -2.654699e-05
## 7      0.76562   1050000    1.1025e+12  0.7658509  4.437259e-05 -2.308816e-04
## 8      0.87487   1200000    1.4400e+12  0.8745930  4.609026e-05  2.770207e-04
## 9      0.98292   1350000    1.8225e+12  0.9831928  4.770597e-05 -2.728402e-04
## 10     1.09146   1500000    2.2500e+12  1.0916505  4.864177e-05 -1.904643e-04
## 11     1.20001   1650000    2.7225e+12  1.1999659  4.864177e-05  4.414850e-05
## 12     1.30822   1800000    3.2400e+12  1.3081390  4.770597e-05  8.099812e-05
## 13     1.41599   1950000    3.8025e+12  1.4161699  4.609026e-05 -1.799154e-04
## 14     1.52399   2100000    4.4100e+12  1.5240586  4.437259e-05 -6.859211e-05
## 15     1.63194   2250000    5.0625e+12  1.6318050  4.354343e-05  1.349680e-04
## 16     1.73947   2400000    5.7600e+12  1.7394092  4.495244e-05  6.076504e-05
## 17     1.84646   2550000    6.5025e+12  1.8468712  4.986859e-05 -4.112011e-04
## 18     1.95392   2700000    7.2900e+12  1.9541909  5.888246e-05 -2.709305e-04
## 19     2.06128   2850000    8.1225e+12  2.0613684  7.185366e-05 -8.842293e-05
## 20     2.16844   3000000    9.0000e+12  2.1684037  8.834303e-05  3.632143e-05
## 21     0.11052    150000    2.2500e+10  0.1104113  8.834303e-05  1.086786e-04
## 22     0.22018    300000    9.0000e+10  0.2200068  7.185366e-05  1.731598e-04
## 23     0.32939    450000    2.0250e+11  0.3294601  5.888246e-05 -7.012218e-05
## 24     0.43886    600000    3.6000e+11  0.4387712  4.986859e-05  8.883271e-05
## 25     0.54798    750000    5.6250e+11  0.5479400  4.495244e-05  4.002444e-05
## 26     0.65739    900000    8.1000e+11  0.6569665  4.354343e-05  4.234530e-04
## 27     0.76596   1050000    1.1025e+12  0.7658509  4.437259e-05  1.091184e-04
## 28     0.87474   1200000    1.4400e+12  0.8745930  4.609026e-05  1.470207e-04
## 29     0.98300   1350000    1.8225e+12  0.9831928  4.770597e-05 -1.928402e-04
## 30     1.09150   1500000    2.2500e+12  1.0916505  4.864177e-05 -1.504643e-04
## 31     1.20004   1650000    2.7225e+12  1.1999659  4.864177e-05  7.414850e-05
## 32     1.30818   1800000    3.2400e+12  1.3081390  4.770597e-05  4.099812e-05
## 33     1.41613   1950000    3.8025e+12  1.4161699  4.609026e-05 -3.991541e-05
## 34     1.52408   2100000    4.4100e+12  1.5240586  4.437259e-05  2.140789e-05
## 35     1.63159   2250000    5.0625e+12  1.6318050  4.354343e-05 -2.150320e-04
## 36     1.73965   2400000    5.7600e+12  1.7394092  4.495244e-05  2.407650e-04
## 37     1.84696   2550000    6.5025e+12  1.8468712  4.986859e-05  8.879887e-05
## 38     1.95445   2700000    7.2900e+12  1.9541909  5.888246e-05  2.590695e-04
## 39     2.06177   2850000    8.1225e+12  2.0613684  7.185366e-05  4.015771e-04
## 40     2.16829   3000000    9.0000e+12  2.1684037  8.834303e-05 -1.136786e-04
##          .hat          .sigma      .cooksd      .std.resid
## 1  0.18538961  0.0002039531  0.1083557670 -1.1951404
```

```
## 2 0.12264183 0.0001922123 0.2518888277 -2.3250603
## 3 0.08235931 0.0002079426 0.0006913290 0.1520138
## 4 0.05907382 0.0002045811 0.0253004370 1.0995244
## 5 0.04800068 0.0002074384 0.0033987136 0.4496893
## 6 0.04503873 0.0002079583 0.0002755909 -0.1324015
## 7 0.04677033 0.0002042395 0.0217256885 -1.1525531
## 8 0.05046138 0.0002025394 0.0340077449 1.3855631
## 9 0.05406129 0.0002026849 0.0356120360 -1.3672481
## 10 0.05620301 0.0002054251 0.0181237925 -0.9555308
## 11 0.05620301 0.0002078697 0.0009737642 0.2214864
## 12 0.05406129 0.0002075440 0.0031385560 0.4058952
## 13 0.05046138 0.0002057188 0.0143446582 -0.8998756
## 14 0.04677033 0.0002076778 0.0019175348 -0.3424095
## 15 0.04503873 0.0002067300 0.0071235449 0.6731448
## 16 0.04800068 0.0002077485 0.0015484646 0.3035330
## 17 0.05907382 0.0001956411 0.0893330479 -2.0660791
## 18 0.08235931 0.0002025961 0.0568463516 -1.3784528
## 19 0.12264183 0.0002074117 0.0098635717 -0.4600943
## 20 0.18538961 0.0002078994 0.0029183068 0.1961365
## 21 0.18538961 0.0002070372 0.0261272044 0.5868666
## 22 0.12264183 0.0002057130 0.0378266955 0.9010087
## 23 0.08235931 0.0002076495 0.0038080074 -0.3567710
## 24 0.05907382 0.0002074468 0.0041691675 0.4463397
## 25 0.04800068 0.0002078952 0.0006718065 0.1999297
## 26 0.04503873 0.0001950675 0.0701204501 2.1119458
## 27 0.04677033 0.0002071719 0.0048527858 0.5447155
## 28 0.05046138 0.0002064820 0.0095787822 0.7353473
## 29 0.05406129 0.0002053659 0.0177899720 -0.9663547
## 30 0.05620301 0.0002063997 0.0113106830 -0.7548568
## 31 0.05620301 0.0002076183 0.0027467977 0.3719919
## 32 0.05406129 0.0002078889 0.0008040960 0.2054485
## 33 0.05046138 0.0002078955 0.0007060488 -0.1996433
## 34 0.04677033 0.0002079755 0.0001867854 0.1068675
## 35 0.04503873 0.0002047490 0.0180817416 -1.0724586
## 36 0.04800068 0.0002039013 0.0243097555 1.2026674
## 37 0.05907382 0.0002074473 0.0041659922 0.4461697
## 38 0.08235931 0.0002030652 0.0519780155 1.3181064
## 39 0.12264183 0.0001953495 0.2034427365 2.0895409
## 40 0.18538961 0.0002069456 0.0285865876 -0.6138667
```

```
load_cell_fit_2_runs <- load_cell_fit_2 %>%
  mutate(
    run = case_when(seq_along(Load) <= 20 ~ "run1",
                     seq_along(Load) > 20 ~ "run2"))

load_cell_fit_2_runs
```

##	Deflection	Load	Load_squared	.fitted	.se.fit	.resid
## 1	0.11019	150000	2.2500e+10	0.1104113	8.834303e-05	-2.213214e-04
## 2	0.21956	300000	9.0000e+10	0.2200068	7.185366e-05	-4.468402e-04
## 3	0.32949	450000	2.0250e+11	0.3294601	5.888246e-05	2.987782e-05
## 4	0.43899	600000	3.6000e+11	0.4387712	4.986859e-05	2.188327e-04
## 5	0.54803	750000	5.6250e+11	0.5479400	4.495244e-05	9.002444e-05
## 6	0.65694	900000	8.1000e+11	0.6569665	4.354343e-05	-2.654699e-05
## 7	0.76562	1050000	1.1025e+12	0.7658509	4.437259e-05	-2.308816e-04

```

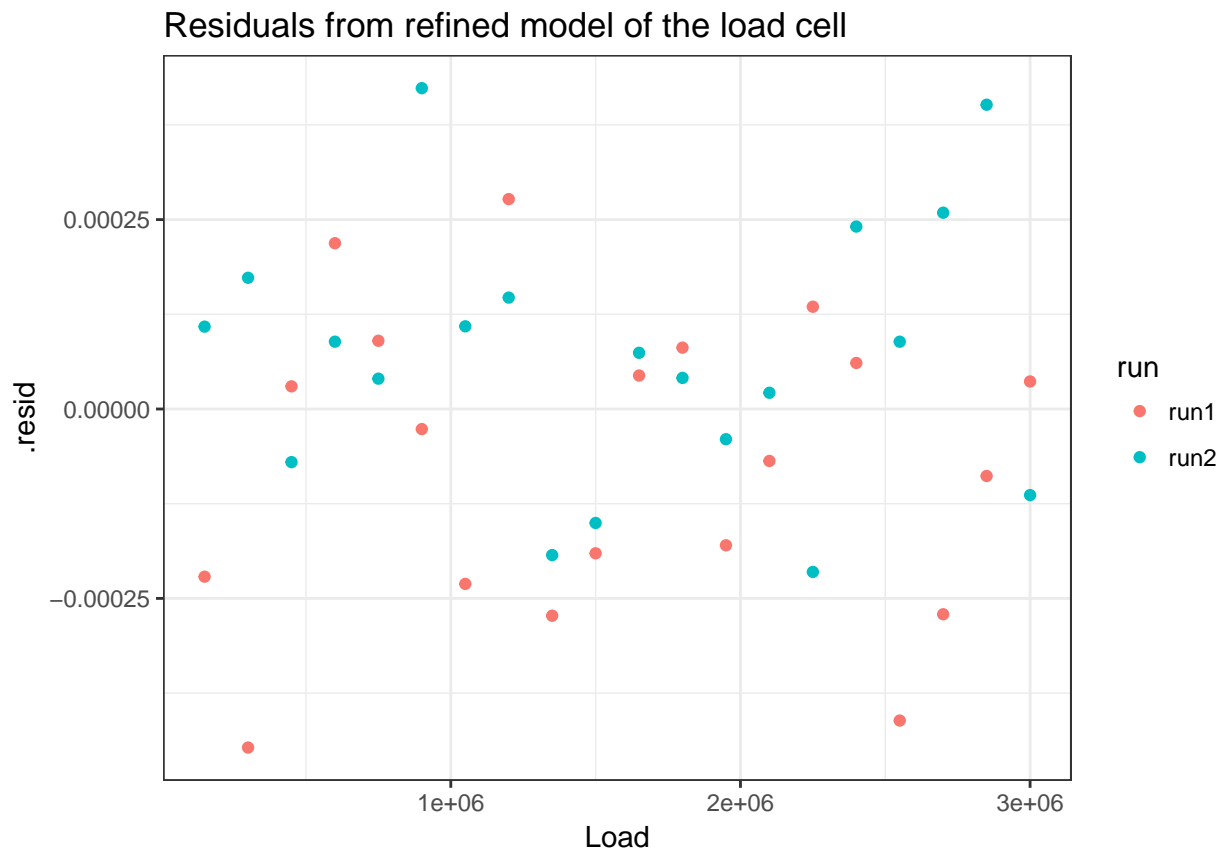
## 8      0.87487 1200000      1.4400e+12 0.8745930 4.609026e-05 2.770207e-04
## 9      0.98292 1350000      1.8225e+12 0.9831928 4.770597e-05 -2.728402e-04
## 10     1.09146 1500000      2.2500e+12 1.0916505 4.864177e-05 -1.904643e-04
## 11     1.20001 1650000      2.7225e+12 1.1999659 4.864177e-05 4.414850e-05
## 12     1.30822 1800000      3.2400e+12 1.3081390 4.770597e-05 8.099812e-05
## 13     1.41599 1950000      3.8025e+12 1.4161699 4.609026e-05 -1.799154e-04
## 14     1.52399 2100000      4.4100e+12 1.5240586 4.437259e-05 -6.859211e-05
## 15     1.63194 2250000      5.0625e+12 1.6318050 4.354343e-05 1.349680e-04
## 16     1.73947 2400000      5.7600e+12 1.7394092 4.495244e-05 6.076504e-05
## 17     1.84646 2550000      6.5025e+12 1.8468712 4.986859e-05 -4.112011e-04
## 18     1.95392 2700000      7.2900e+12 1.9541909 5.888246e-05 -2.709305e-04
## 19     2.06128 2850000      8.1225e+12 2.0613684 7.185366e-05 -8.842293e-05
## 20     2.16844 3000000      9.0000e+12 2.1684037 8.834303e-05 3.632143e-05
## 21     0.11052 150000      2.2500e+10 0.1104113 8.834303e-05 1.086786e-04
## 22     0.22018 300000      9.0000e+10 0.2200068 7.185366e-05 1.731598e-04
## 23     0.32939 450000      2.0250e+11 0.3294601 5.888246e-05 -7.012218e-05
## 24     0.43886 600000      3.6000e+11 0.4387712 4.986859e-05 8.883271e-05
## 25     0.54798 750000      5.6250e+11 0.5479400 4.495244e-05 4.002444e-05
## 26     0.65739 900000      8.1000e+11 0.6569665 4.354343e-05 4.234530e-04
## 27     0.76596 1050000     1.1025e+12 0.7658509 4.437259e-05 1.091184e-04
## 28     0.87474 1200000     1.4400e+12 0.8745930 4.609026e-05 1.470207e-04
## 29     0.98300 1350000     1.8225e+12 0.9831928 4.770597e-05 -1.928402e-04
## 30     1.09150 1500000     2.2500e+12 1.0916505 4.864177e-05 -1.504643e-04
## 31     1.20004 1650000     2.7225e+12 1.1999659 4.864177e-05 7.414850e-05
## 32     1.30818 1800000     3.2400e+12 1.3081390 4.770597e-05 4.099812e-05
## 33     1.41613 1950000     3.8025e+12 1.4161699 4.609026e-05 -3.991541e-05
## 34     1.52408 2100000     4.4100e+12 1.5240586 4.437259e-05 2.140789e-05
## 35     1.63159 2250000     5.0625e+12 1.6318050 4.354343e-05 -2.150320e-04
## 36     1.73965 2400000     5.7600e+12 1.7394092 4.495244e-05 2.407650e-04
## 37     1.84696 2550000     6.5025e+12 1.8468712 4.986859e-05 8.879887e-05
## 38     1.95445 2700000     7.2900e+12 1.9541909 5.888246e-05 2.590695e-04
## 39     2.06177 2850000     8.1225e+12 2.0613684 7.185366e-05 4.015771e-04
## 40     2.16829 3000000     9.0000e+12 2.1684037 8.834303e-05 -1.136786e-04
##      .hat      .sigma      .cooksd .std.resid run
## 1 0.18538961 0.0002039531 0.1083557670 -1.1951404 run1
## 2 0.12264183 0.0001922123 0.2518888277 -2.3250603 run1
## 3 0.08235931 0.0002079426 0.0006913290 0.1520138 run1
## 4 0.05907382 0.0002045811 0.0253004370 1.0995244 run1
## 5 0.04800068 0.0002074384 0.0033987136 0.4496893 run1
## 6 0.04503873 0.0002079583 0.0002755909 -0.1324015 run1
## 7 0.04677033 0.0002042395 0.0217256885 -1.1525531 run1
## 8 0.05046138 0.0002025394 0.0340077449 1.3855631 run1
## 9 0.05406129 0.0002026849 0.0356120360 -1.3672481 run1
## 10 0.05620301 0.0002054251 0.0181237925 -0.9555308 run1
## 11 0.05620301 0.0002078697 0.0009737642 0.2214864 run1
## 12 0.05406129 0.0002075440 0.0031385560 0.4058952 run1
## 13 0.05046138 0.0002057188 0.0143446582 -0.8998756 run1
## 14 0.04677033 0.0002076778 0.0019175348 -0.3424095 run1
## 15 0.04503873 0.0002067300 0.0071235449 0.6731448 run1
## 16 0.04800068 0.0002077485 0.0015484646 0.3035330 run1
## 17 0.05907382 0.0001956411 0.0893330479 -2.0660791 run1
## 18 0.08235931 0.0002025961 0.0568463516 -1.3784528 run1
## 19 0.12264183 0.0002074117 0.0098635717 -0.4600943 run1
## 20 0.18538961 0.0002078994 0.0029183068 0.1961365 run1

```

```
## 21 0.18538961 0.0002070372 0.0261272044 0.5868666 run2
## 22 0.12264183 0.0002057130 0.0378266955 0.9010087 run2
## 23 0.08235931 0.0002076495 0.0038080074 -0.3567710 run2
## 24 0.05907382 0.0002074468 0.0041691675 0.4463397 run2
## 25 0.04800068 0.0002078952 0.0006718065 0.1999297 run2
## 26 0.04503873 0.0001950675 0.0701204501 2.1119458 run2
## 27 0.04677033 0.0002071719 0.0048527858 0.5447155 run2
## 28 0.05046138 0.0002064820 0.0095787822 0.7353473 run2
## 29 0.05406129 0.0002053659 0.0177899720 -0.9663547 run2
## 30 0.05620301 0.0002063997 0.0113106830 -0.7548568 run2
## 31 0.05620301 0.0002076183 0.0027467977 0.3719919 run2
## 32 0.05406129 0.0002078889 0.0008040960 0.2054485 run2
## 33 0.05046138 0.0002078955 0.0007060488 -0.1996433 run2
## 34 0.04677033 0.0002079755 0.0001867854 0.1068675 run2
## 35 0.04503873 0.0002047490 0.0180817416 -1.0724586 run2
## 36 0.04800068 0.0002039013 0.0243097555 1.2026674 run2
## 37 0.05907382 0.0002074473 0.0041659922 0.4461697 run2
## 38 0.08235931 0.0002030652 0.0519780155 1.3181064 run2
## 39 0.12264183 0.0001953495 0.2034427365 2.0895409 run2
## 40 0.18538961 0.0002069456 0.0285865876 -0.6138667 run2
```

#### 4.3.4.6 EDA of load cell data by run

```
ggplot(load_cell_fit_2_runs) +
  geom_point(aes(Load, .resid, colour = run)) +
  ggtitle("Residuals from refined model of the load cell") +
  theme_bw()
```



## 4.4 Applying models to multiple datasets

### 4.4.1 Revisting the Ascombe dataset

```
x_anscombe <- anscombe %>% # results will be stored into a new object x_anscombe; we start with the o
dplyr::select(x1, x2, x3, x4) %>% # select the columns we want to work with
rename(group1 = x1, group2 = x2, group3 = x3, group4 = x4) %>% # rename the values using a generic he
gather(key = group, value = x_values, group1, group2, group3, group4) # gather the columns into rows
```

```
x_anscombe
```

```
##      group x_values
## 1  group1      10
## 2  group1       8
## 3  group1      13
## 4  group1       9
## 5  group1      11
## 6  group1      14
## 7  group1       6
## 8  group1       4
## 9  group1      12
## 10 group1       7
## 11 group1       5
## 12 group2      10
## 13 group2       8
```

```
## 14 group2      13
## 15 group2       9
## 16 group2     11
## 17 group2     14
## 18 group2       6
## 19 group2       4
## 20 group2     12
## 21 group2       7
## 22 group2       5
## 23 group3     10
## 24 group3       8
## 25 group3     13
## 26 group3       9
## 27 group3     11
## 28 group3     14
## 29 group3       6
## 30 group3       4
## 31 group3     12
## 32 group3       7
## 33 group3       5
## 34 group4       8
## 35 group4       8
## 36 group4       8
## 37 group4       8
## 38 group4       8
## 39 group4       8
## 40 group4       8
## 41 group4     19
## 42 group4       8
## 43 group4       8
## 44 group4       8
```

```
y_anscombe <- anscombe %>%
  dplyr::select(y1, y2, y3, y4) %>%
  gather(key = group, value = y_values, y1, y2, y3, y4) %>% # I don't need to rename the columns as I w
  dplyr::select(y_values)
```

```
y_anscombe
```

```
##      y_values
## 1      8.04
## 2      6.95
## 3      7.58
## 4      8.81
## 5      8.33
## 6      9.96
## 7      7.24
## 8      4.26
## 9     10.84
## 10     4.82
## 11     5.68
## 12     9.14
## 13     8.14
## 14     8.74
## 15     8.77
```

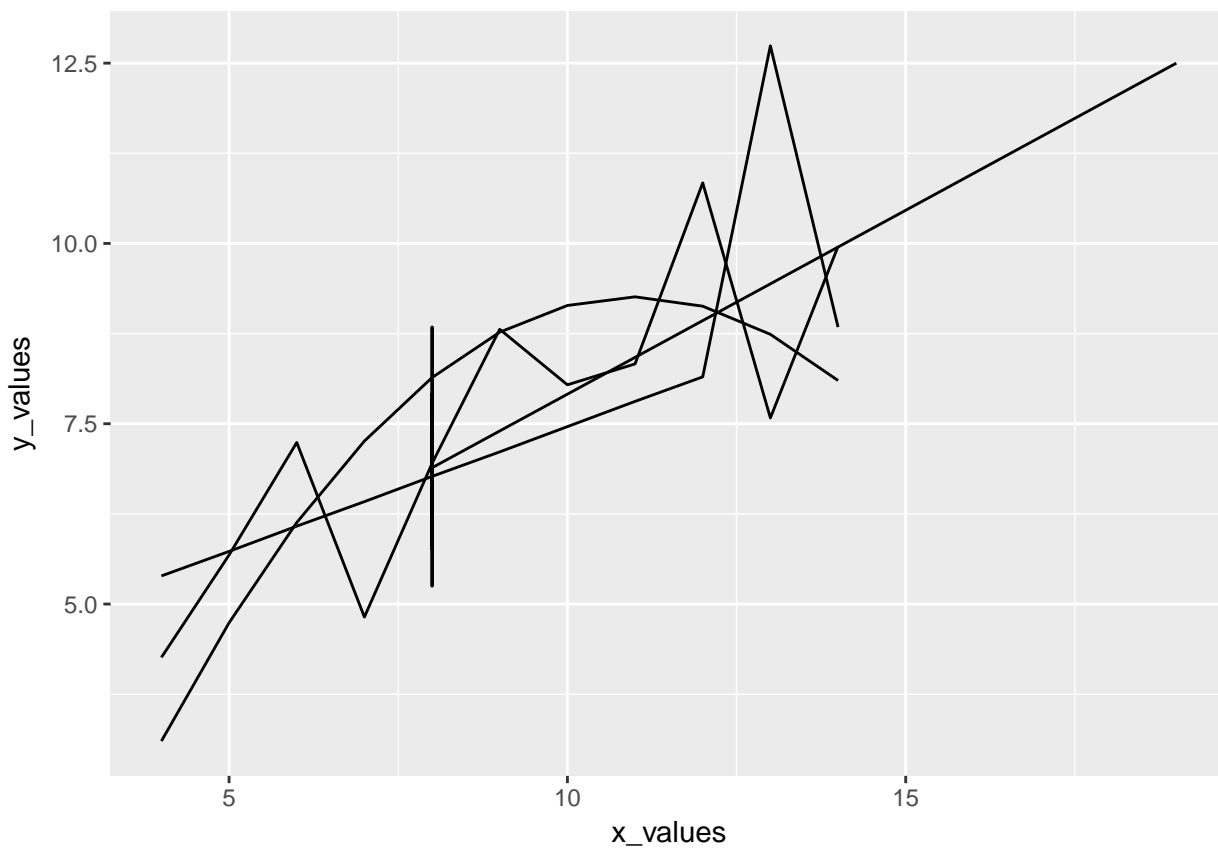
```
## 16      9.26
## 17      8.10
## 18      6.13
## 19      3.10
## 20      9.13
## 21      7.26
## 22      4.74
## 23      7.46
## 24      6.77
## 25     12.74
## 26      7.11
## 27      7.81
## 28      8.84
## 29      6.08
## 30      5.39
## 31      8.15
## 32      6.42
## 33      5.73
## 34      6.58
## 35      5.76
## 36      7.71
## 37      8.84
## 38      8.47
## 39      7.04
## 40      5.25
## 41     12.50
## 42      5.56
## 43      7.91
## 44      6.89
```

```
anscombe_tidy <- bind_cols(x_anscombe, y_anscombe)
anscombe_tidy
```

```
##      group x_values y_values
## 1  group1      10      8.04
## 2  group1       8      6.95
## 3  group1      13      7.58
## 4  group1       9      8.81
## 5  group1      11      8.33
## 6  group1      14      9.96
## 7  group1       6      7.24
## 8  group1       4      4.26
## 9  group1      12     10.84
## 10 group1       7      4.82
## 11 group1       5      5.68
## 12 group2      10      9.14
## 13 group2       8      8.14
## 14 group2      13      8.74
## 15 group2       9      8.77
## 16 group2      11      9.26
## 17 group2      14      8.10
## 18 group2       6      6.13
## 19 group2       4      3.10
## 20 group2      12      9.13
## 21 group2       7      7.26
```

```
## 22 group2      5      4.74
## 23 group3     10      7.46
## 24 group3      8      6.77
## 25 group3     13     12.74
## 26 group3      9      7.11
## 27 group3     11      7.81
## 28 group3     14      8.84
## 29 group3      6      6.08
## 30 group3      4      5.39
## 31 group3     12      8.15
## 32 group3      7      6.42
## 33 group3      5      5.73
## 34 group4      8      6.58
## 35 group4      8      5.76
## 36 group4      8      7.71
## 37 group4      8      8.84
## 38 group4      8      8.47
## 39 group4      8      7.04
## 40 group4      8      5.25
## 41 group4     19     12.50
## 42 group4      8      5.56
## 43 group4      8      7.91
## 44 group4      8      6.89
```

```
ggplot(anscombe_tidy, aes(x_values, y_values)) +
  geom_line(aes(group = group))
```



In chapter 1, we constructed models for each group; however, for large datasets, we'd like to be able to



streamline this process.

Following the example from chapter 11 of Hadley Wickham:

```
anscombe_models <- anscombe_tidy %>%
  group_by(group) %>%
  do(mod = lm(y_values ~ x_values, data = ., na.action = na.exclude
    )) %>%
  ungroup()

anscombe_models

## # A tibble: 4 x 2
##   group mod
## * <chr> <list>
## 1 group1 <S3: lm>
## 2 group2 <S3: lm>
## 3 group3 <S3: lm>
## 4 group4 <S3: lm>
```

#### 4.4.2 Model-level summaries

```
model_summary <- anscombe_models %>%
  rowwise() %>%
  glance(mod)

model_summary

## # A tibble: 4 x 12
## # Groups:   group [4]
##   group r.squared adj.r.squared sigma statistic p.value    df logLik  AIC
##   <chr>   <dbl>         <dbl> <dbl>    <dbl>   <dbl> <int> <dbl> <dbl>
## 1 grou~    0.667           0.629  1.24     18.0 0.00217     2  -16.8  39.7
## 2 grou~    0.666           0.629  1.24     18.0 0.00218     2  -16.8  39.7
## 3 grou~    0.666           0.629  1.24     18.0 0.00218     2  -16.8  39.7
## 4 grou~    0.667           0.630  1.24     18.0 0.00216     2  -16.8  39.7
## # ... with 3 more variables: BIC <dbl>, deviance <dbl>, df.residual <int>
```

#### 4.4.3 Coefficient-level summaries

```
coefficient_summary <- anscombe_models %>%
  rowwise() %>%
  tidy(mod)

coefficient_summary

## # A tibble: 8 x 6
## # Groups:   group [4]
##   group term          estimate std.error statistic p.value
##   <chr> <chr>         <dbl>    <dbl>    <dbl>   <dbl>
## 1 group1 (Intercept)    3.00     1.12     2.67 0.0257
## 2 group1 x_values       0.500    0.118     4.24 0.00217
## 3 group2 (Intercept)    3.00     1.13     2.67 0.0258
```

```
## 4 group2 x_values      0.500      0.118      4.24 0.00218
## 5 group3 (Intercept)   3.00      1.12      2.67 0.0256
## 6 group3 x_values      0.500      0.118      4.24 0.00218
## 7 group4 (Intercept)   3.00      1.12      2.67 0.0256
## 8 group4 x_values      0.500      0.118      4.24 0.00216
```

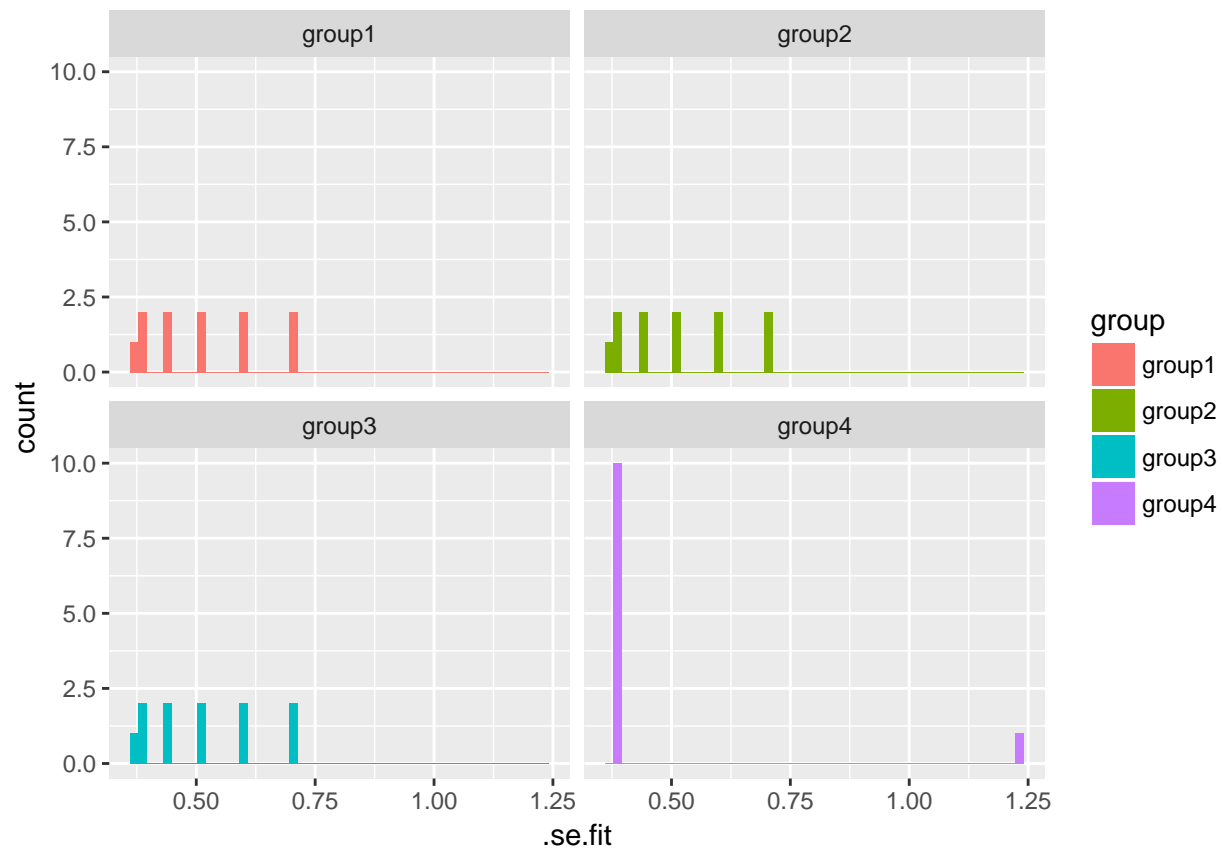
#### 4.4.4 Observation Data

```
observation_summary <- anscombe_models %>%
  rowwise() %>%
  augment(mod)

observation_summary
```

```
## # A tibble: 44 x 10
## # Groups:   group [4]
##   group y_values x_values .fitted .se.fit .resid .hat .sigma .cooksd
##   <chr>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>
## 1 group1     8.04     10.     8.00   0.391   0.0390  0.100    1.31  6.14e-5
## 2 group1     6.95      8.     7.00   0.391  -0.0508  0.100    1.31  1.04e-4
## 3 group1     7.58     13.     9.50   0.601  -1.92    0.236    1.06  4.89e-1
## 4 group1     8.81      9.     7.50   0.373   1.31    0.0909   1.22  6.16e-2
## 5 group1     8.33     11.     8.50   0.441  -0.171   0.127    1.31  1.60e-3
## 6 group1     9.96     14.    10.0   0.698  -0.0414  0.318    1.31  3.83e-4
## 7 group1     7.24      6.     6.00   0.514   1.24    0.173    1.22  1.27e-1
## 8 group1     4.26      4.     5.00   0.698  -0.740   0.318    1.27  1.23e-1
## 9 group1    10.8     12.     9.00   0.514   1.84    0.173    1.10  2.79e-1
## 10 group1     4.82      7.     6.50   0.441  -1.68    0.127    1.15  1.54e-1
## # ... with 34 more rows, and 1 more variable: .std.resid <dbl>

ggplot(observation_summary, aes(.se.fit, fill = group)) +
  geom_histogram(bins = 50) +
  facet_wrap(~ group)
```



Having model information for each dataset can make the overall analysis much more efficient.



# Chapter 5

## Process Improvement

### 5.1 Packages used in this chapter

```
library(tidyverse)
library(ggplot2)
library(broom)
```

### 5.2 Case Studies

#### 5.2.1 Eddy current probe sensitivity

Eddy current probe sensitivity

##### 5.2.1.1 Background

The data for this case study is a subset of a study performed by Capobianco, Splett, and Iyer. Capobianco was a member of the NIST Electromagnetics Division and Splett and Iyer were members of the NIST Statistical Engineering Division at the time of this study.

The goal of this project is to develop a nondestructive portable device for detecting cracks and fractures in metals. A primary application would be the detection of defects in airplane wings. The internal mechanism of the detector would be for sensing crack-induced changes in the detector's electromagnetic field, which would in turn result in changes in the impedance level of the detector. This change of impedance is termed “sensitivity” and it is a sub-goal of this experiment to maximize such sensitivity as the detector is moved from an unflawed region to a flawed region on the metal.

##### 5.2.1.2 Statistical goals

The case study illustrates the analysis of a 23 full factorial experimental design. The specific statistical goals of the experiment are: (1) Determine the important factors that affect sensitivity. (2) Determine the settings that maximize sensitivity. (3) Determine a prediction equation that functionally relates sensitivity to various factors.

## 5.2.1.3 Data

```
eddy_probe <- read_table2("NIST data/SPLETT3.DAT",
                          skip = 25, col_names = FALSE, col_types = "diiiii") %>%
  rename(probe_impedance = X1, number_turns = X2, winding_distance = X3, wire_gauge = X4, run_sequence = X5)
eddy_probe
```

```
## # A tibble: 8 x 5
##   probe_impedance number_turns winding_distance wire_gauge run_sequence
##         <dbl>         <int>         <int>         <int>         <int>
## 1         1.70             -1             -1             -1             2
## 2         4.57              1             -1             -1             8
## 3         0.550            -1              1             -1             3
## 4         3.39              1              1             -1             6
## 5         1.51            -1             -1              1             7
## 6         4.59              1             -1              1             1
## 7         0.670            -1              1              1             4
## 8         4.29              1              1              1             5
```

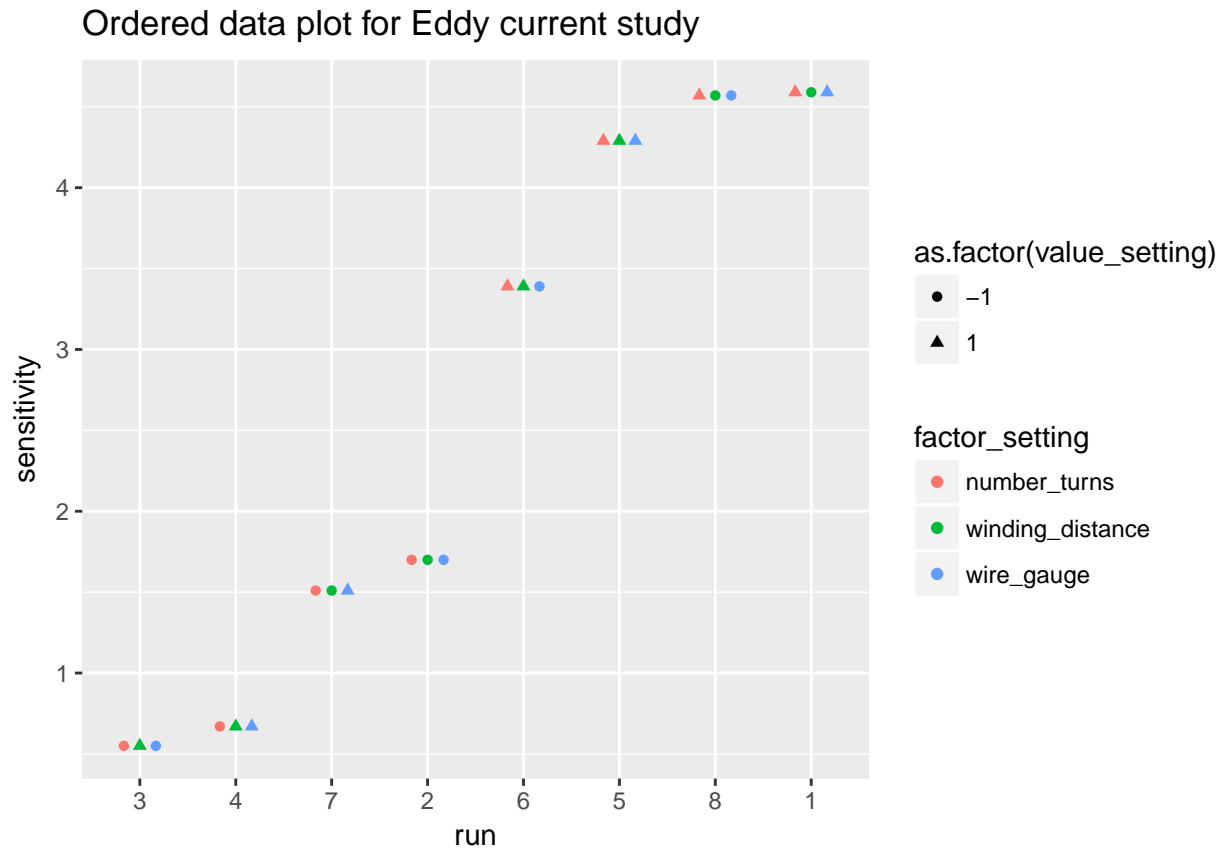
## 5.2.1.4 Ordered data plot

There are several different ways we could structure an ordered data plot; below is an example.

```
eddy_probe_tidy <- eddy_probe %>%
  gather(key = factor_setting, value = value_setting, number_turns, winding_distance, wire_gauge)
eddy_probe_tidy
```

```
## # A tibble: 24 x 4
##   probe_impedance run_sequence factor_setting value_setting
##         <dbl>         <int> <chr>         <int>
## 1         1.70             2 number_turns      -1
## 2         4.57             8 number_turns       1
## 3         0.550            3 number_turns     -1
## 4         3.39             6 number_turns       1
## 5         1.51             7 number_turns     -1
## 6         4.59             1 number_turns       1
## 7         0.670            4 number_turns     -1
## 8         4.29             5 number_turns       1
## 9         1.70             2 winding_distance  -1
## 10        4.57             8 winding_distance  -1
## # ... with 14 more rows
```

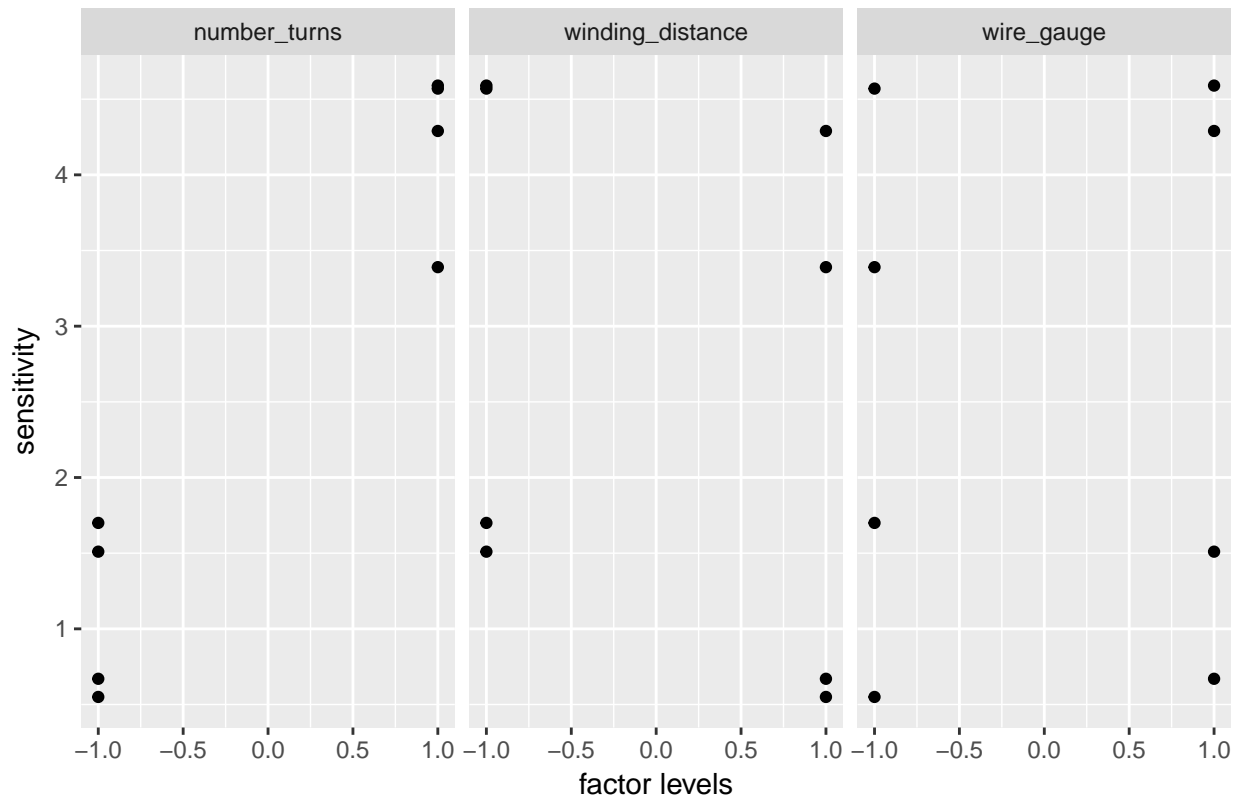
```
ggplot(eddy_probe_tidy) +
  geom_point(aes(reorder(run_sequence, probe_impedance), probe_impedance, colour = factor_setting, shape = factor_setting)) +
  labs(title = "Ordered data plot for Eddy current study", y = "sensitivity", x = "run")
```



#### 5.2.1.5 DOE scatter plot

```
ggplot(eddy_probe_tidy) +
  geom_point(aes(value_setting, probe_impedance)) +
  facet_wrap(~factor_setting) +
  labs(title = "DOE scatter plot for Eddy current data", y = "sensitivity", x = "factor levels")
```

DOE scatter plot for Eddy current data



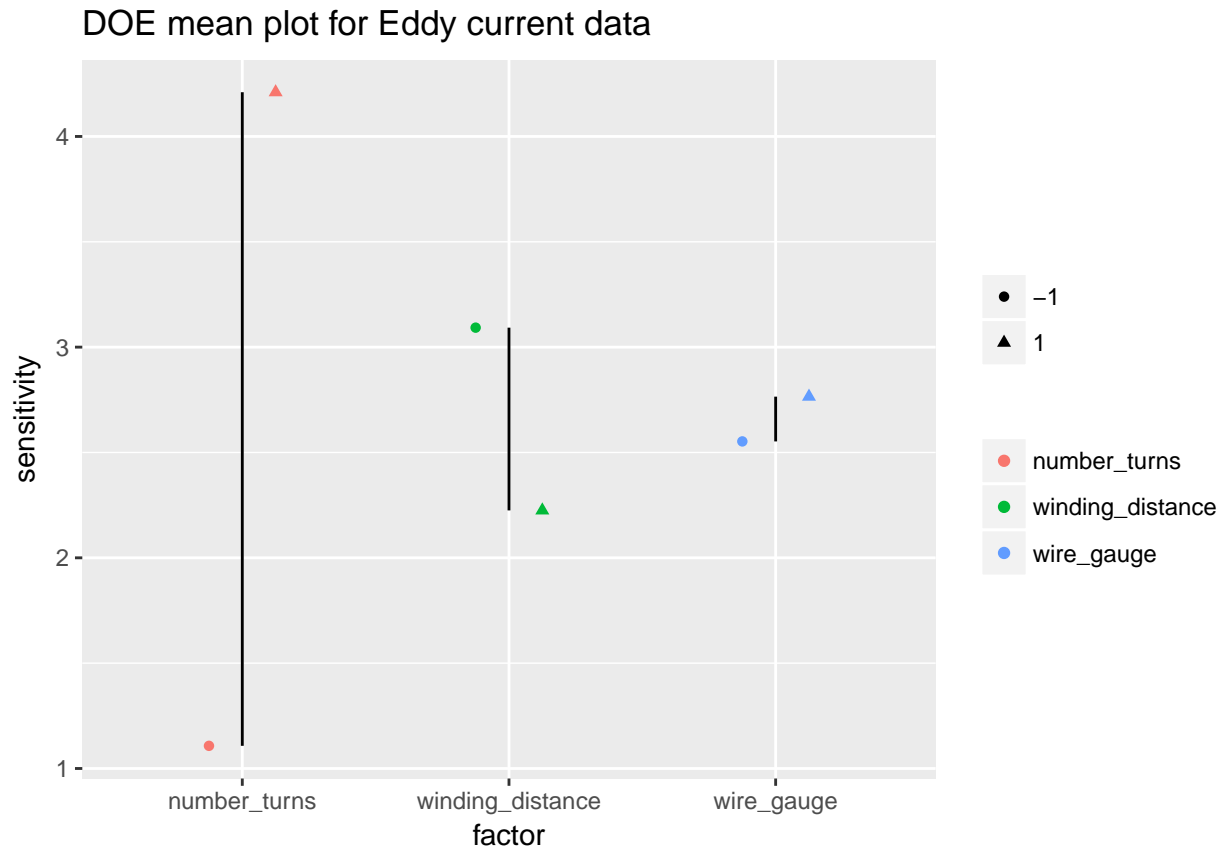
#### 5.2.1.6 DOE mean plot

```
eddy_probe_means <- eddy_probe_tidy %>%
  group_by(factor_setting, value_setting) %>%
  summarise(n = n(), average_factor = mean(probe_impedance))
eddy_probe_means
```

```
## # A tibble: 6 x 4
## # Groups:   factor_setting [?]
##   factor_setting value_setting     n average_factor
##   <chr>          <int> <int>         <dbl>
## 1 number_turns      -1     4          1.11
## 2 number_turns       1     4          4.21
## 3 winding_distance  -1     4          3.09
## 4 winding_distance   1     4          2.22
## 5 wire_gauge        -1     4          2.55
## 6 wire_gauge         1     4          2.76
```

```
ggplot(eddy_probe_means, aes(factor_setting, average_factor)) +
  geom_point(aes(colour = factor_setting, shape = as.factor(value_setting)), position = position_dodge()) +
  geom_line(aes(group = factor_setting)) +
  labs(title = "DOE mean plot for Eddy current data", y = "sensitivity", x = "factor") +
  theme(legend.title = element_blank())
```





#### 5.2.1.7 DOE interaction plot for eddy current data

```
eddy_probe_interaction <- lm(average_factor ~ factor_setting, data = eddy_probe_means)
summary(eddy_probe_interaction)
```

```
##
## Call:
## lm(formula = average_factor ~ factor_setting, data = eddy_probe_means)
##
## Residuals:
##      1      2      3      4      5      6
## -1.5512  1.5513  0.4337 -0.4338 -0.1062  0.1062
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)      2.659e+00  9.320e-01   2.853   0.065 .
## factor_settingwinding_distance -8.802e-16  1.318e+00   0.000   1.000
## factor_settingwire_gauge      -2.220e-16  1.318e+00   0.000   1.000
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.318 on 3 degrees of freedom
## Multiple R-squared:  1.892e-31, Adjusted R-squared:  -0.6667
## F-statistic: 2.838e-31 on 2 and 3 DF,  p-value: 1
```



## Chapter 6

# Process Monitoring

### 6.1 Packages used in this chapter

```
library(magrittr) # used for %$% pipe
library(tidyverse)
library(ggplot2)
library(broom)
```

### 6.2 Case Studies

#### 6.2.1 Lithography Process Example

Lithography process example

##### 6.2.1.1 Background

One of the assumptions in using classical Shewhart SPC charts is that the only source of variation is from part to part (or within subgroup variation). This is the case for most continuous processing situations. However, many of today's processing situations have different sources of variation. The semiconductor industry is one of the areas where the processing creates multiple sources of variation.

In semiconductor processing, the basic experimental unit is a silicon wafer. Operations are performed on the wafer, but individual wafers can be grouped multiple ways. In the diffusion area, up to 150 wafers are processed in one time in a diffusion tube. In the etch area, single wafers are processed individually. In the lithography area, the light exposure is done on sub-areas of the wafer. There are many times during the production of a computer chip where the experimental unit varies and thus there are different sources of variation in this batch processing environment.

The following is a case study of a lithography process. Five sites are measured on each wafer, three wafers are measured in a cassette (typically a grouping of 24 - 25 wafers) and thirty cassettes of wafers are used in the study. The width of a line is the measurement under study. There are two line width variables. The first is the original data and the second has been cleaned up somewhat. This case study uses the raw data. The entire data table is 450 rows long with six columns.

## 6.2.1.2 Data

```
litho <- read_table2("NIST data/monitor-6.6.1.1.dat",
  skip = 4, col_names = FALSE) %>%
  rename(cassette = X1, wafer = X2, site = X3, raw_linewidth = X4, run_number = X5, cleaned_linewidth =

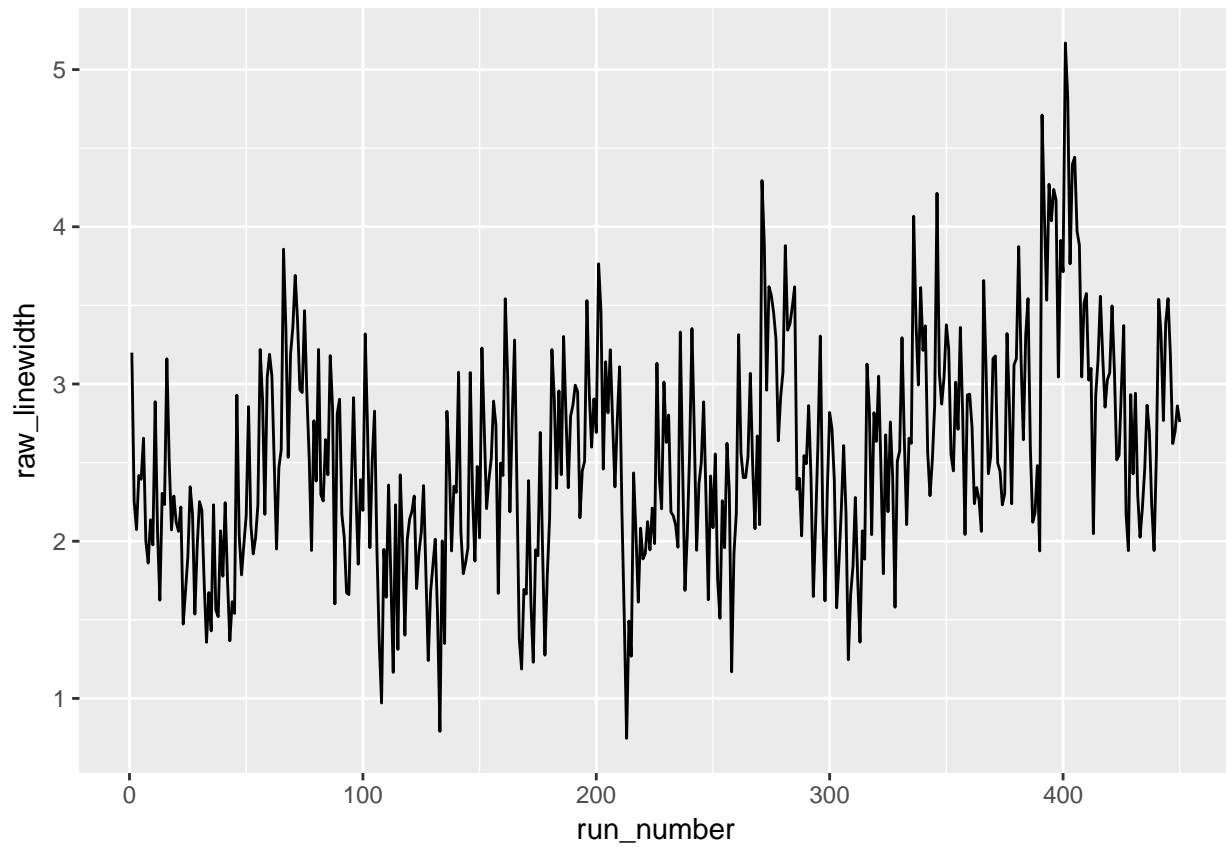
## Parsed with column specification:
## cols(
##   X1 = col_integer(),
##   X2 = col_integer(),
##   X3 = col_character(),
##   X4 = col_double(),
##   X5 = col_integer(),
##   X6 = col_double()
## )

litho

## # A tibble: 450 x 6
##   cassette wafer site raw_linewidth run_number cleaned_linewidth
##   <int> <int> <chr>      <dbl>      <int>      <dbl>
## 1         1     1 Top         3.20         1         3.20
## 2         1     1 Lef         2.25         2         2.25
## 3         1     1 Cen         2.07         3         2.07
## 4         1     1 Rgt         2.42         4         2.41
## 5         1     1 Bot         2.39         5         2.38
## 6         1     2 Top         2.65         6         2.64
## 7         1     2 Lef         2.00         7         1.99
## 8         1     2 Cen         1.86         8         1.85
## 9         1     2 Rgt         2.14         9         2.12
## 10        1     2 Bot         1.98        10         1.96
## # ... with 440 more rows
```

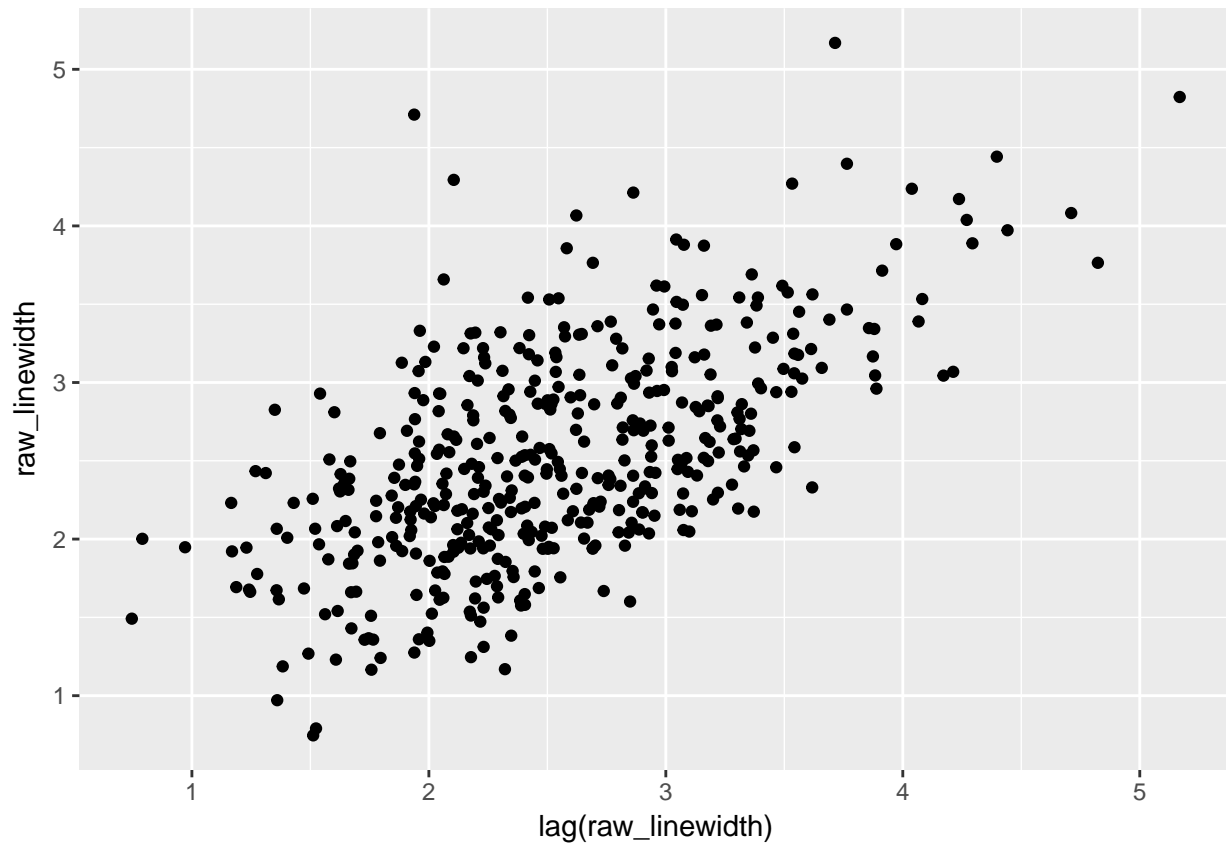
## 6.2.1.3 Generate some simple plots

```
ggplot(litho) +
  geom_line(aes(run_number, raw_linewidth))
```



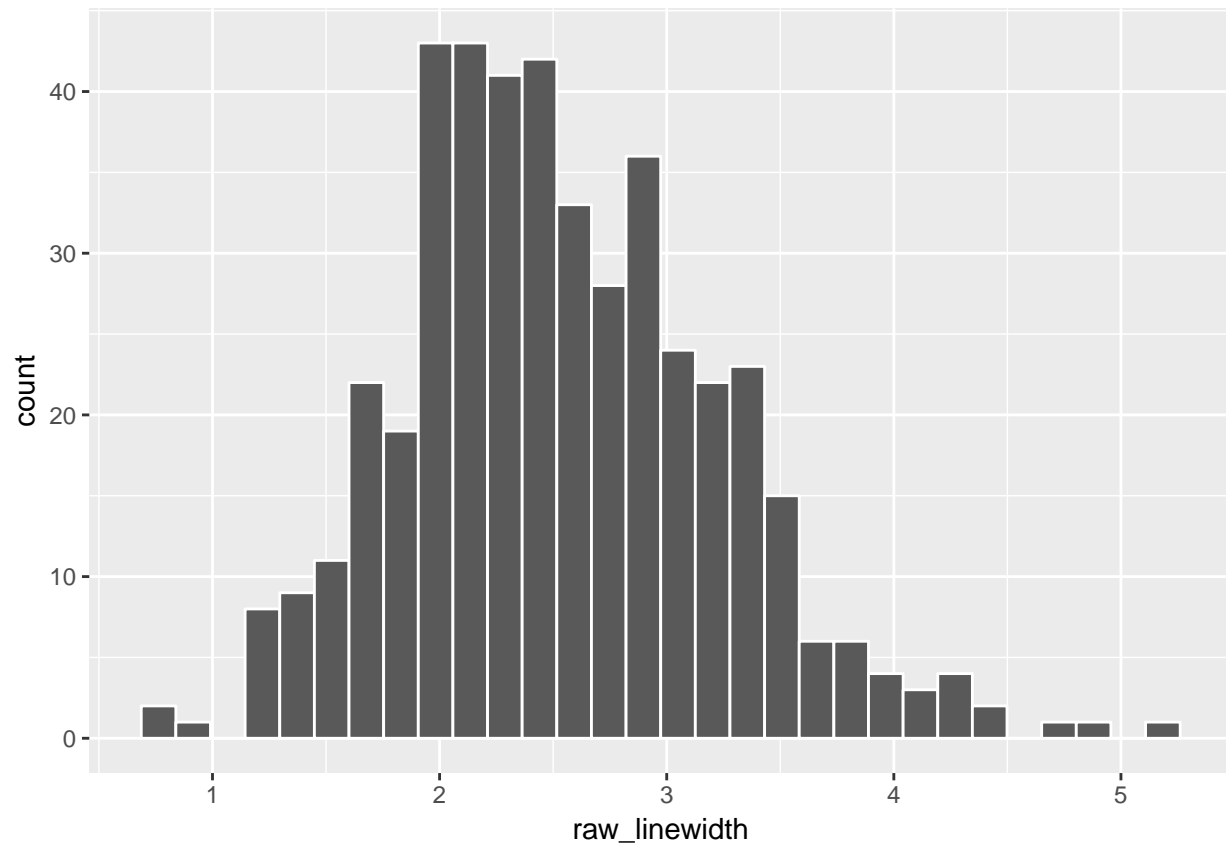
```
ggplot(litho) +  
  geom_point(aes(lag(raw_linewidth), raw_linewidth))
```

```
## Warning: Removed 1 rows containing missing values (geom_point).
```

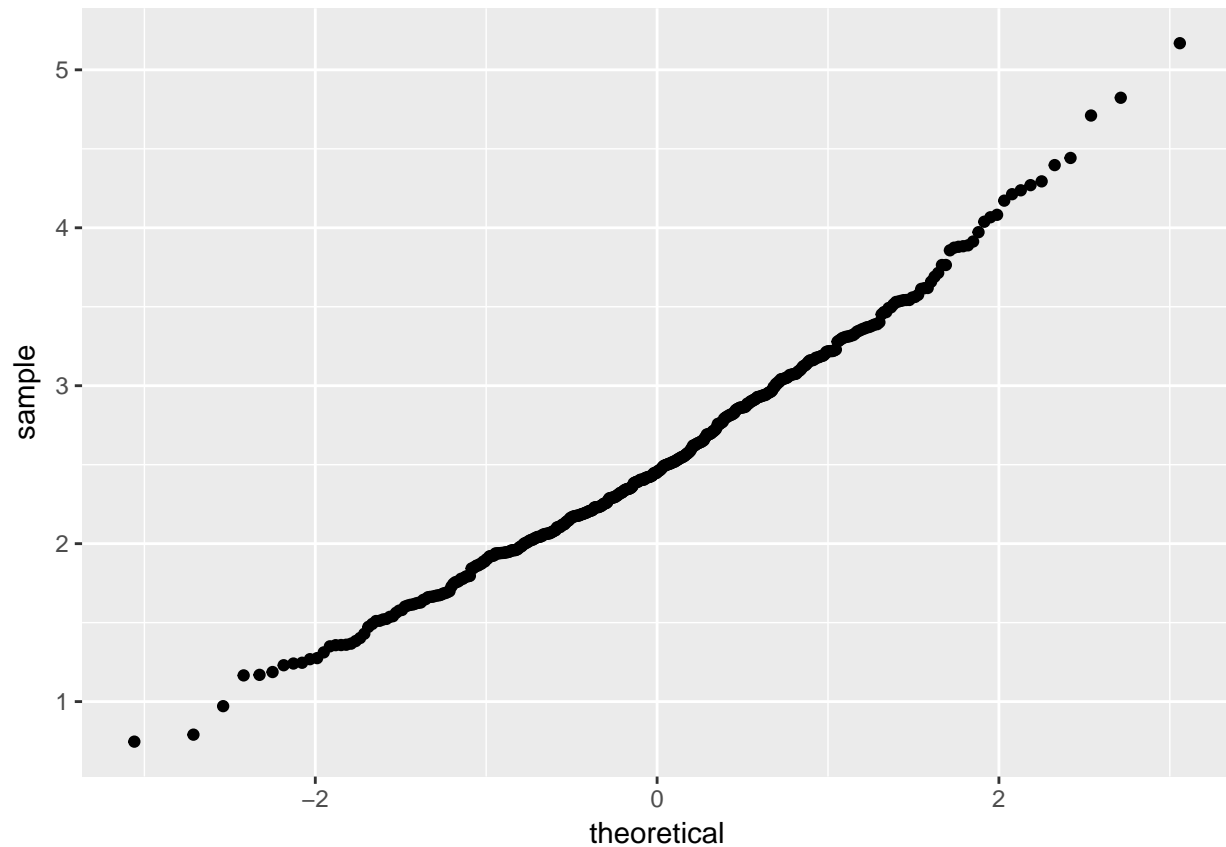


```
ggplot(litho) +  
  geom_histogram(aes(raw_linewidth), colour = "white")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(litho) +  
  geom_qq(aes(sample = raw_linewidth))
```



#### 6.2.1.4 Summarise the raw linewidth and cleaned linesidh data

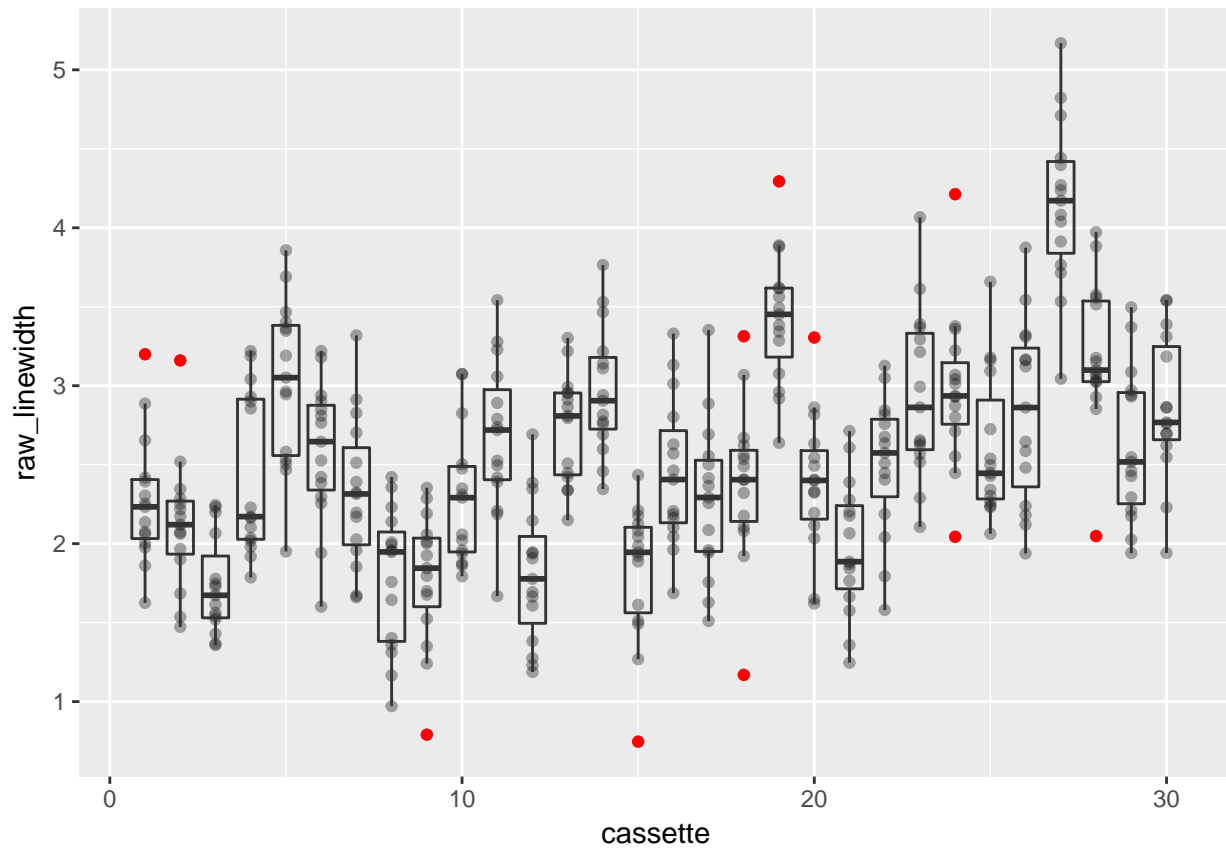
```
litho %>%
  dplyr::select(raw_linewidth, cleaned_linewidth) %>%
  summary()
```

```
## raw_linewidth cleaned_linewidth
## Min. :0.7465 Min. :0.3205
## 1st Qu.:2.0505 1st Qu.:1.6476
## Median :2.4533 Median :2.0367
## Mean :2.5323 Mean :2.0813
## 3rd Qu.:2.9697 3rd Qu.:2.4856
## Max. :5.1687 Max. :4.3667
```

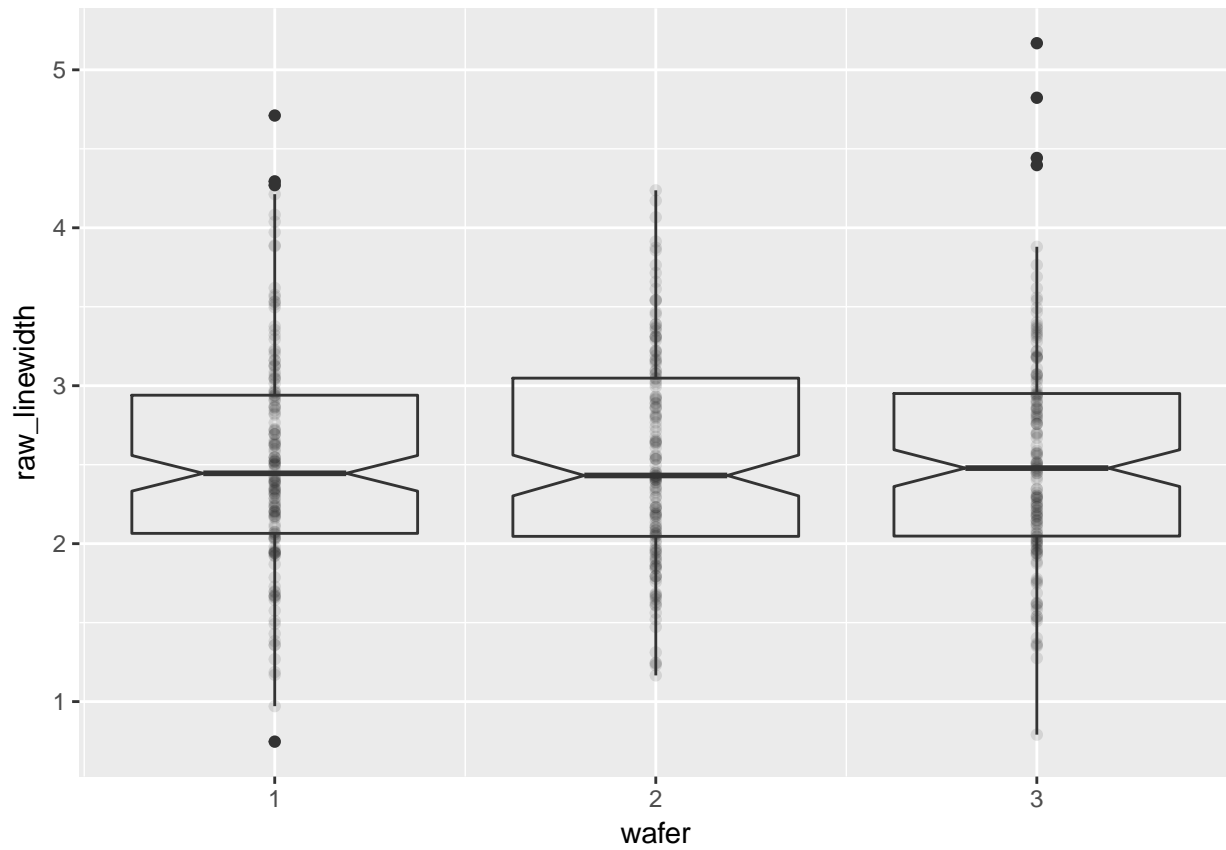
#### 6.2.1.5 Plot the response against individual factors

```
ggplot(litho) +
  geom_point(aes(cassette, raw_linewidth), alpha = 1/3) +
  geom_boxplot(aes(cassette, raw_linewidth, group = cassette), alpha = 0, outlier.alpha = 1, outlier.colour = "red")
```

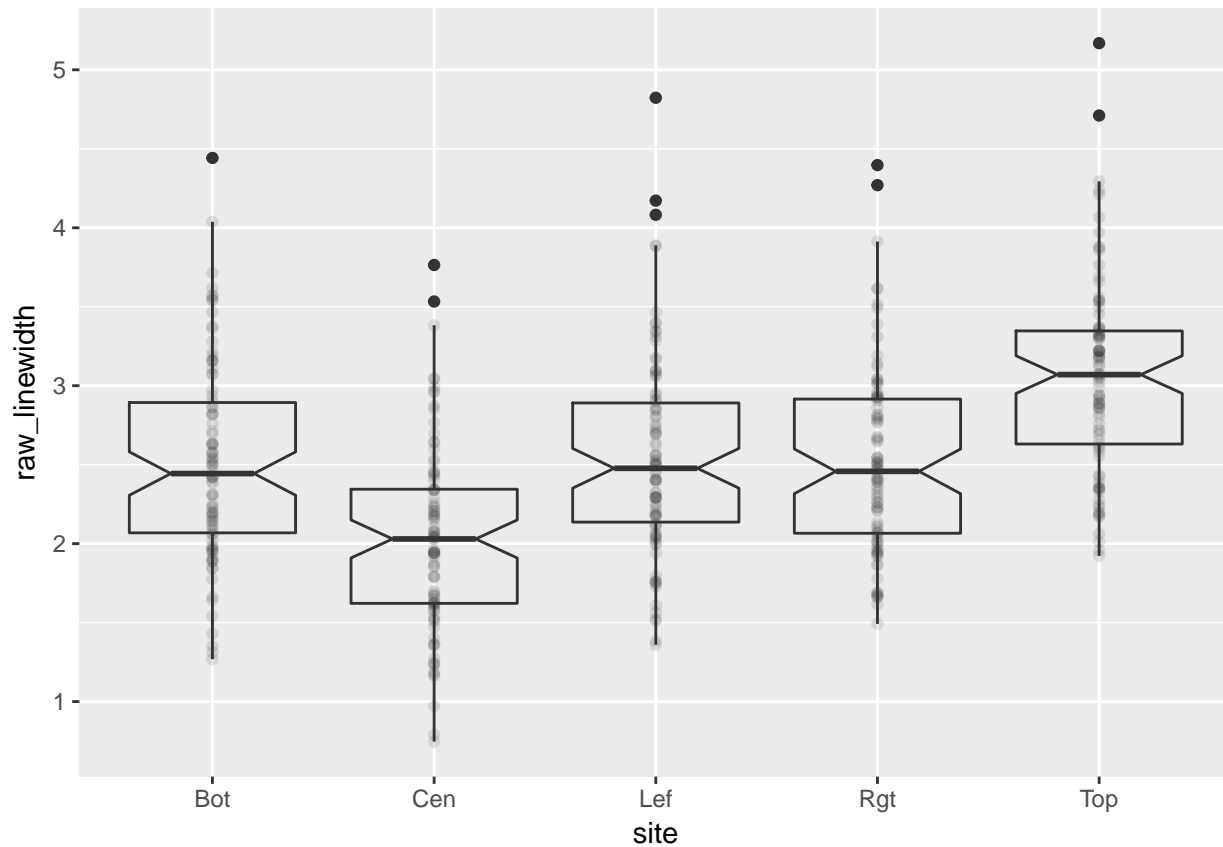




```
ggplot(litho) +  
  geom_point(aes(wafer, raw_linewidth), alpha = 1/10) +  
  geom_boxplot(aes(wafer, raw_linewidth, group = wafer), alpha = 0, notch = TRUE, outlier.alpha = 1)
```



```
ggplot(litho) +  
  geom_point(aes(site, raw_linewidth), alpha = 1/10) +  
  geom_boxplot(aes(site, raw_linewidth), alpha = 0, notch = TRUE, outlier.alpha = 1)
```



### 6.2.1.6 DOE plots

We need to gather the factors in to a single column

```
litho_DOE <- litho %>%
  gather(`cassette`, `wafer`, `site`, key = DOE_factors, value = "value")
litho_DOE
```

```
## # A tibble: 1,350 x 5
##   raw_linewidth run_number cleaned_linewidth DOE_factors value
##         <dbl>      <int>          <dbl> <chr>      <chr>
## 1         3.20         1             3.20 cassette 1
## 2         2.25         2             2.25 cassette 1
## 3         2.07         3             2.07 cassette 1
## 4         2.42         4             2.41 cassette 1
## 5         2.39         5             2.38 cassette 1
## 6         2.65         6             2.64 cassette 1
## 7         2.00         7             1.99 cassette 1
## 8         1.86         8             1.85 cassette 1
## 9         2.14         9             2.12 cassette 1
## 10        1.98        10             1.96 cassette 1
## # ... with 1,340 more rows
```

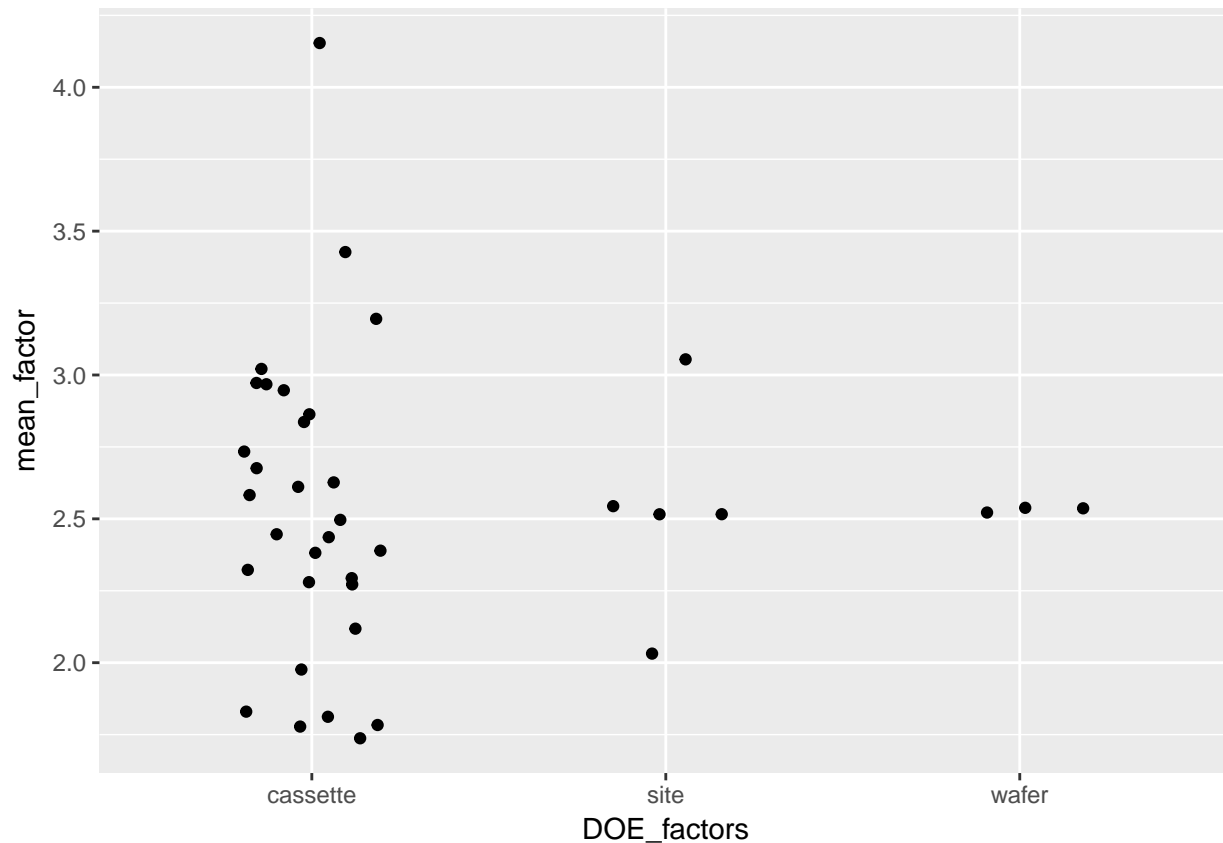
```
litho_group <- litho_DOE %>%
  group_by(DOE_factors, value)
litho_group
```

```
## # A tibble: 1,350 x 5
## # Groups:   DOE_factors, value [38]
##   raw_linewidth run_number cleaned_linewidth DOE_factors value
##   <dbl>         <int>         <dbl> <chr>         <chr>
## 1      3.20           1           3.20 cassette      1
## 2      2.25           2           2.25 cassette      1
## 3      2.07           3           2.07 cassette      1
## 4      2.42           4           2.41 cassette      1
## 5      2.39           5           2.38 cassette      1
## 6      2.65           6           2.64 cassette      1
## 7      2.00           7           1.99 cassette      1
## 8      1.86           8           1.85 cassette      1
## 9      2.14           9           2.12 cassette      1
## 10     1.98          10           1.96 cassette      1
## # ... with 1,340 more rows
```

```
litho_summary <- litho_group %>%
  summarise(mean_factor = mean(raw_linewidth), count = n())
litho_summary
```

```
## # A tibble: 38 x 4
## # Groups:   DOE_factors [?]
##   DOE_factors value mean_factor count
##   <chr>         <chr>         <dbl> <int>
## 1 cassette      1           2.27    15
## 2 cassette     10           2.29    15
## 3 cassette     11           2.68    15
## 4 cassette     12           1.81    15
## 5 cassette     13           2.73    15
## 6 cassette     14           2.97    15
## 7 cassette     15           1.83    15
## 8 cassette     16           2.45    15
## 9 cassette     17           2.28    15
## 10 cassette    18           2.39    15
## # ... with 28 more rows
```

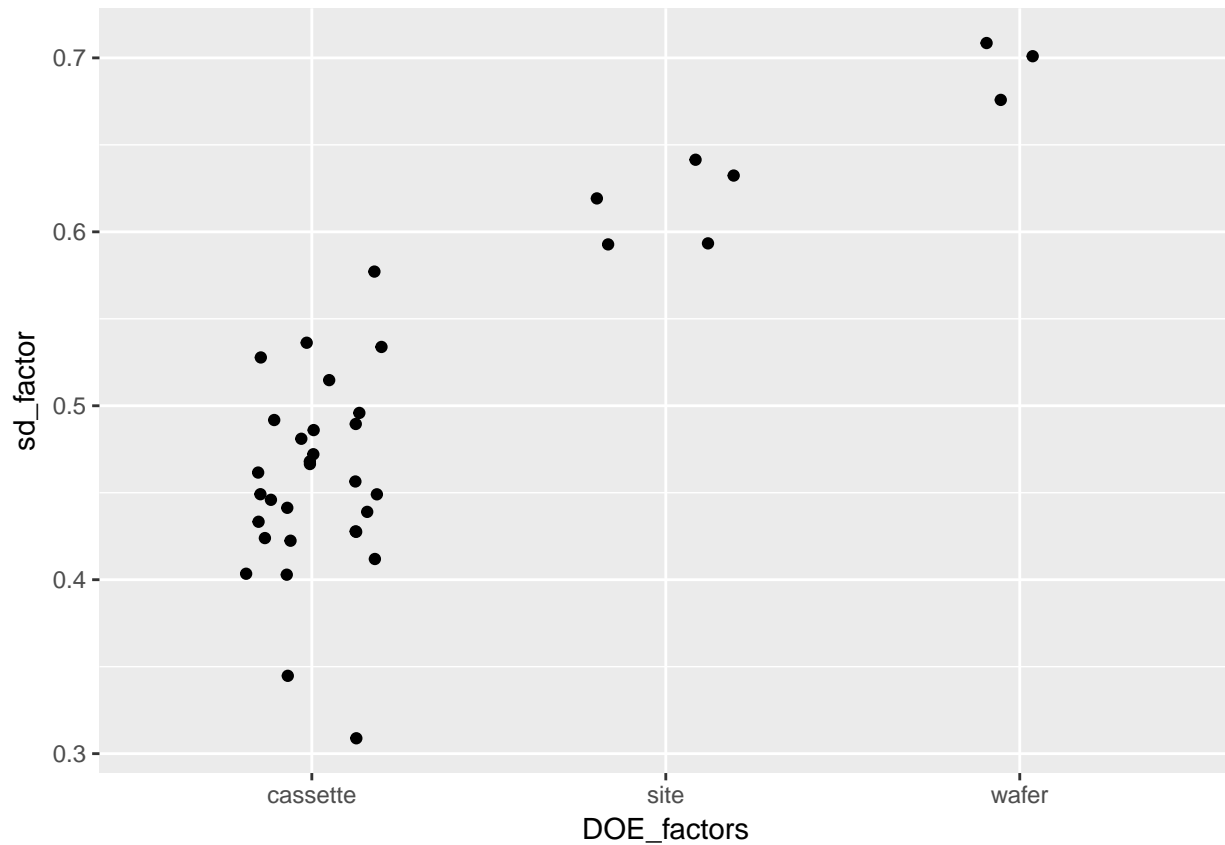
```
ggplot(litho_summary) +
  geom_jitter(aes(DOE_factors, mean_factor), width = 0.2)
```



```
litho_summary_sd <- litho_group %>%
  summarise(sd_factor = sd(raw_linewidth), count = n())
litho_summary_sd
```

```
## # A tibble: 38 x 4
## # Groups:   DOE_factors [?]
##   DOE_factors value sd_factor count
##   <chr>      <chr>    <dbl> <int>
## 1 cassette    1      0.403    15
## 2 cassette   10      0.428    15
## 3 cassette   11      0.486    15
## 4 cassette   12      0.449    15
## 5 cassette   13      0.345    15
## 6 cassette   14      0.403    15
## 7 cassette   15      0.433    15
## 8 cassette   16      0.466    15
## 9 cassette   17      0.492    15
## 10 cassette  18      0.496    15
## # ... with 28 more rows
```

```
ggplot(litho_summary_sd) +
  geom_jitter(aes(DOE_factors, sd_factor), width = 0.2)
```



### 6.2.1.7 Subgroup analysis

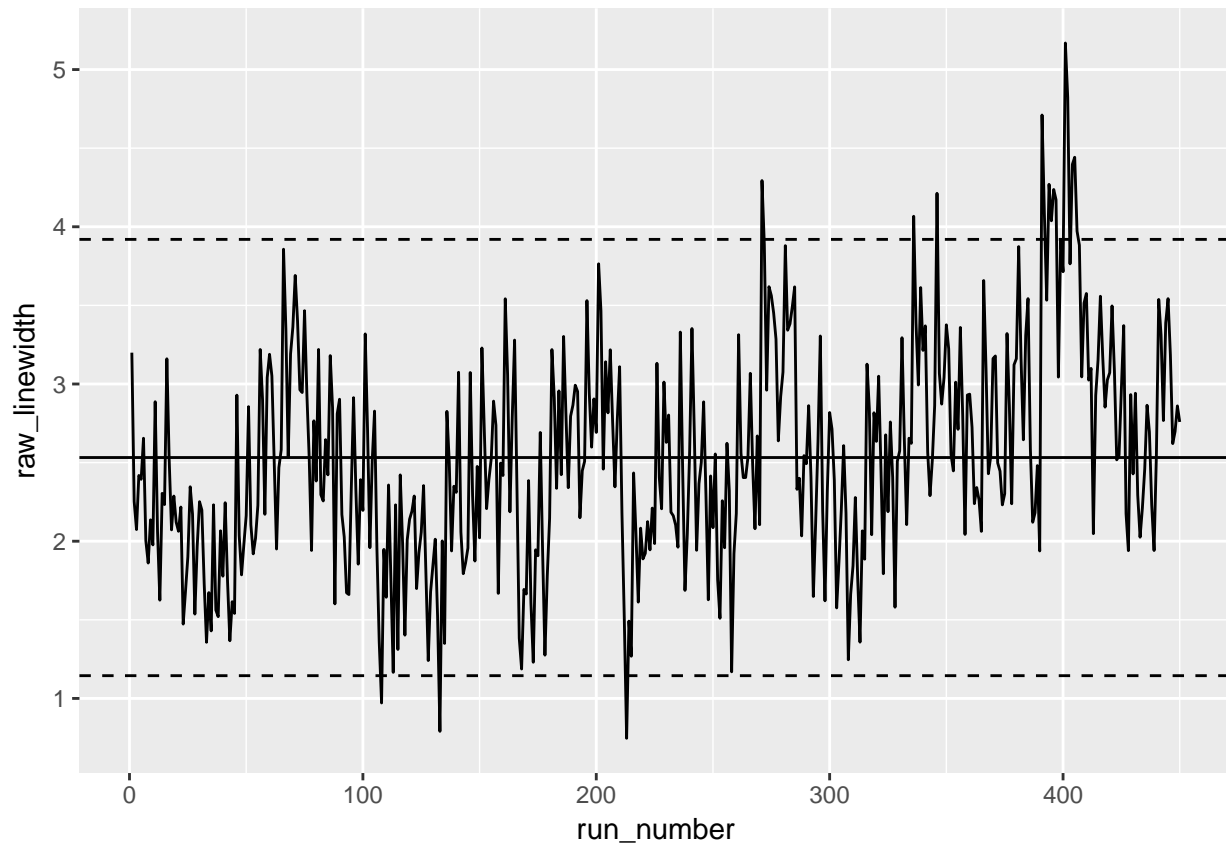
#### 6.2.1.7.1 Run chart

The chart below adds the mean and control limits based on the standard deviation of the data.

```
sd_lw <- litho %$%
  sd(raw_linewidth)

mean_lw <- litho %$%
  mean(raw_linewidth)

ggplot(litho) +
  geom_line(aes(run_number, raw_linewidth)) +
  geom_hline(yintercept = mean_lw + 2*sd_lw, linetype = "dashed") +
  geom_hline(yintercept = mean_lw - 2*sd_lw, linetype = "dashed") +
  geom_hline(yintercept = mean_lw)
```



#### 6.2.1.7.2 Summarise by wafer

```
litho_wafer <- litho %>%
  group_by(cassette, wafer) %>%
  summarise(wafer_mean = mean(raw_linewidth), wafer_sd = sd(raw_linewidth)) %>%
  rowid_to_column(var = "wafer_number") %>%
  ungroup()
```

```
litho_wafer
```

```
## # A tibble: 90 x 5
##   wafer_number cassette wafer wafer_mean wafer_sd
##   <int>      <int> <int>    <dbl>    <dbl>
## 1         1         1     1      2.47     0.431
## 2         2         1     2      2.13     0.311
## 3         3         1     3      2.22     0.456
## 4         4         2     1      2.43     0.443
## 5         5         2     2      1.87     0.296
## 6         6         2     3      2.05     0.322
## 7         7         3     1      1.68     0.331
## 8         8         3     2      1.83     0.311
## 9         9         3     3      1.70     0.333
## 10        10        4     1      2.18     0.441
## # ... with 80 more rows
```

#### 6.2.1.7.3 Wafer stats

```
sd_wafer <- litho_wafer %$%
  sd(wafer_mean)

rms_sd_wafer <- litho_wafer %>%
  dplyr::select(wafer_sd) %>%
  mutate(sd_squared = wafer_sd^2) %$%
  sqrt(mean(sd_squared))

mean_wafer_sd <- litho_wafer %$%
  mean(wafer_sd)

mean_wafer_sd
```

```
## [1] 0.407502
```

```
sd_wafer
```

```
## [1] 0.5862159
```

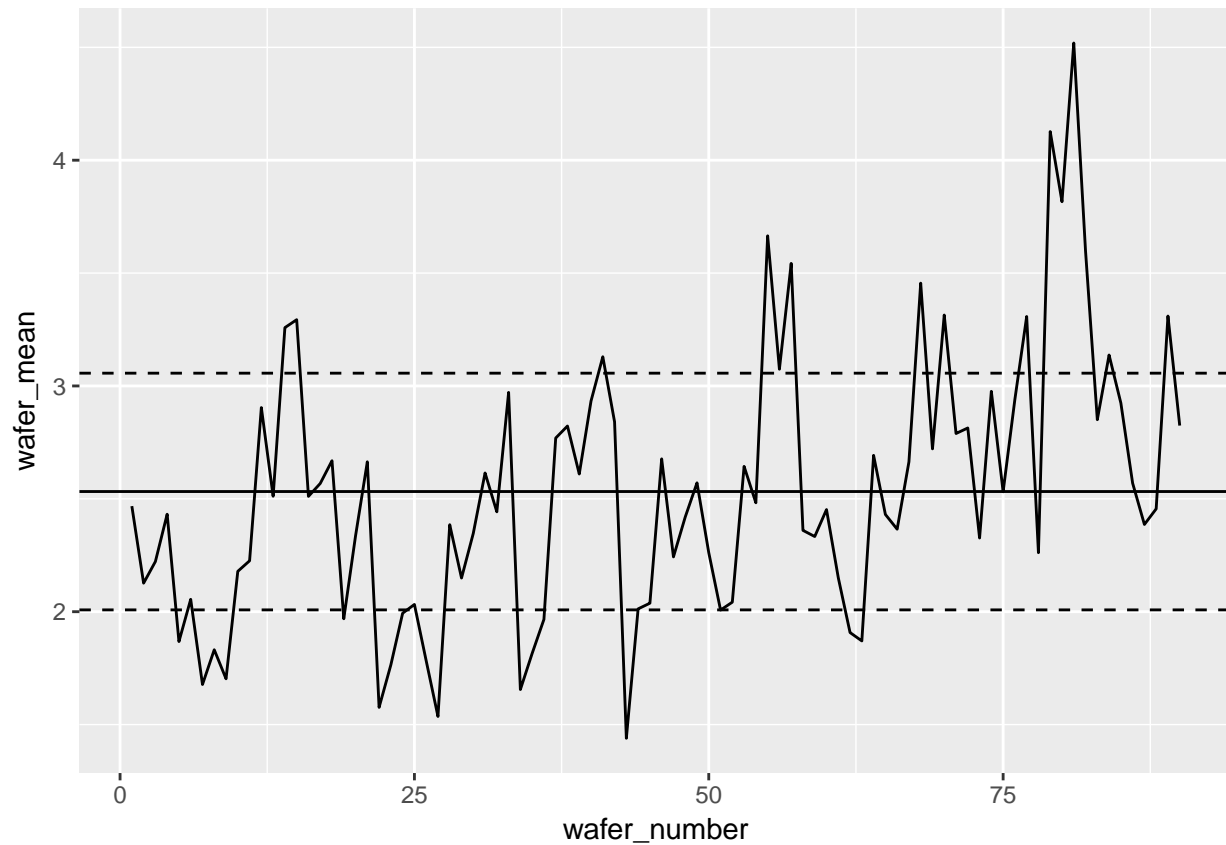
```
rms_sd_wafer
```

```
## [1] 0.4189227
```

#### 6.2.1.7.4 Wafer mean control chart

```
ggplot(litho_wafer) +
  geom_line(aes(wafer_number, wafer_mean)) +
  geom_hline(yintercept = mean_lw + 2*sd_wafer/sqrt(5), linetype = "dashed") +
  geom_hline(yintercept = mean_lw - 2*sd_wafer/sqrt(5), linetype = "dashed") +
  geom_hline(yintercept = mean_lw)
```



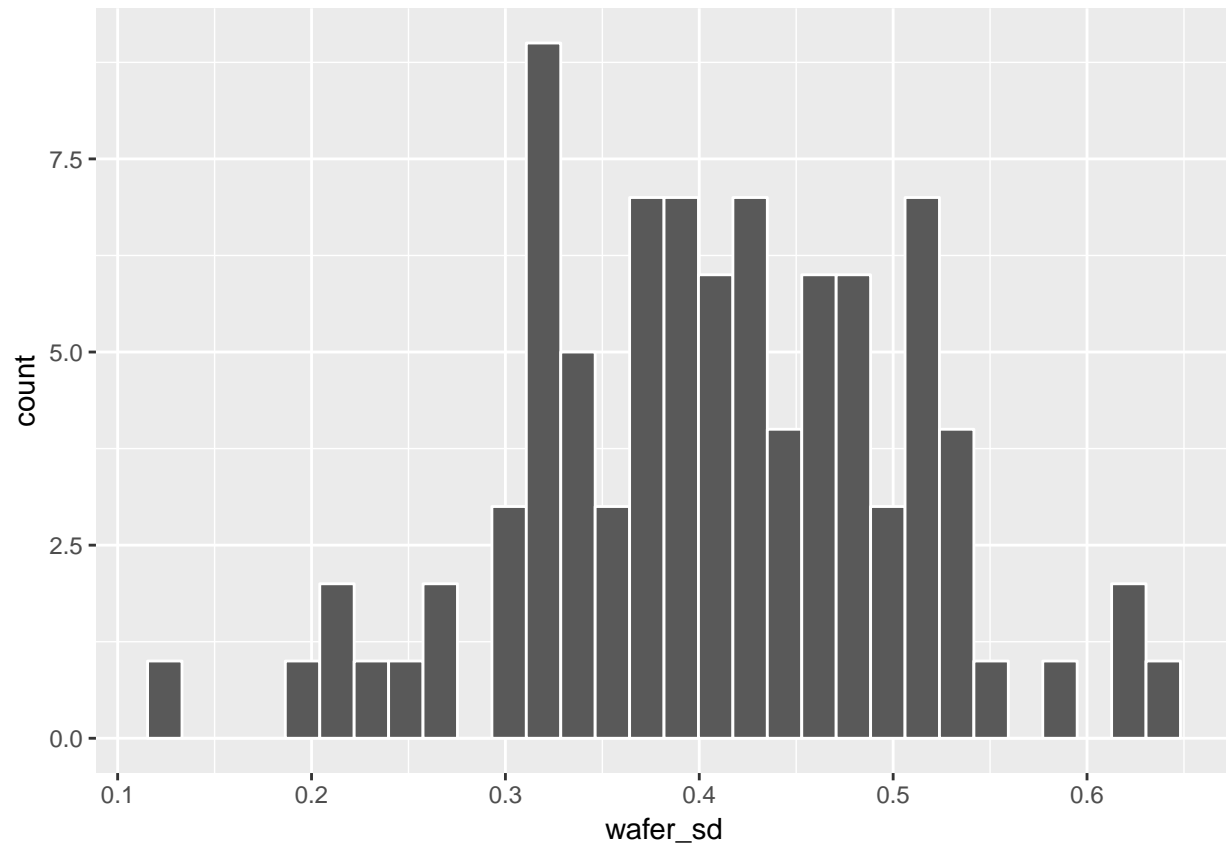


#### 6.2.1.7.5 SD control chart by wafer

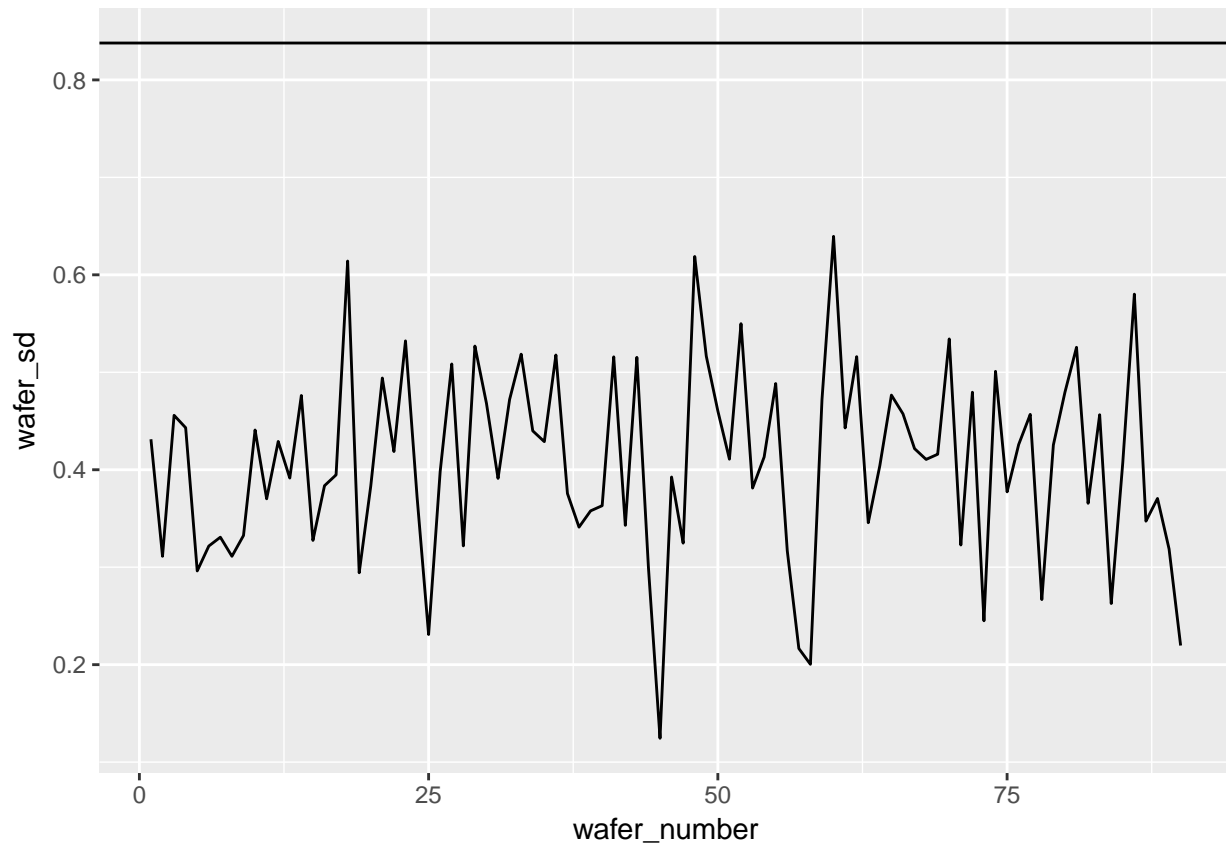
Using the methods from (2.2.3.1. Control chart for standard)[<https://www.itl.nist.gov/div898/handbook/mpc/section2/mpc231.htm>] we can construct an UCL for the standard deviations

```
ggplot(litho_wafer) +  
  geom_histogram(aes(wafer_sd), colour = "white")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```
ggplot(litho_wafer) +  
  geom_line(aes(wafer_number, wafer_sd)) +  
  geom_hline(yintercept = 2*rms_sd_wafer)
```



#### 6.2.1.7.6 Summarise by cassette

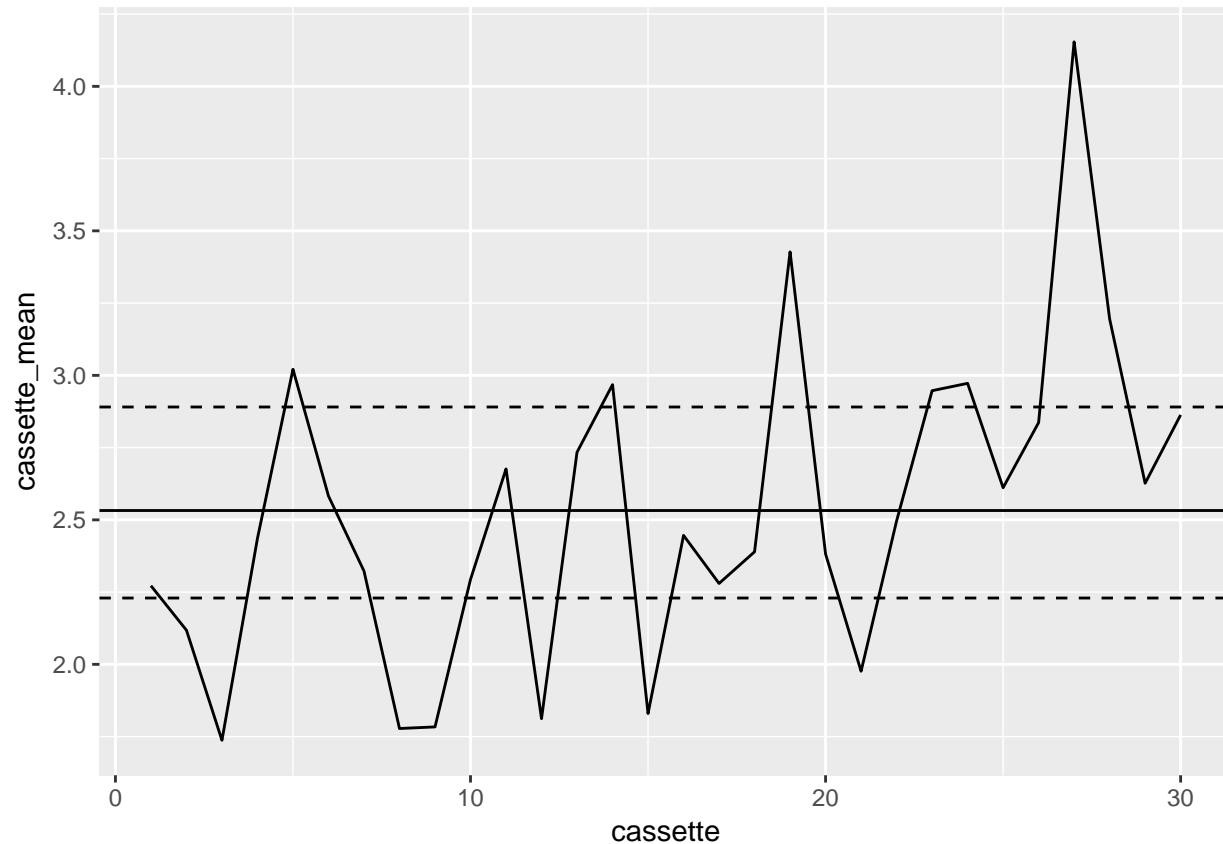
```
litho_cassette <- litho %>%
  group_by(cassette) %>%
  summarise(cassette_mean = mean(raw_linewidth), cassette_sd = sd(raw_linewidth)) %>%
  ungroup()
```

```
litho_cassette
```

```
## # A tibble: 30 x 3
##   cassette cassette_mean cassette_sd
##   <int>         <dbl>         <dbl>
## 1         1         2.27         0.403
## 2         2         2.12         0.412
## 3         3         1.74         0.309
## 4         4         2.44         0.515
## 5         5         3.02         0.528
## 6         6         2.58         0.446
## 7         7         2.32         0.472
## 8         8         1.78         0.449
## 9         9         1.78         0.422
## 10        10         2.29         0.428
## # ... with 20 more rows
```

#### 6.2.1.7.7 Mean control chart by cassette

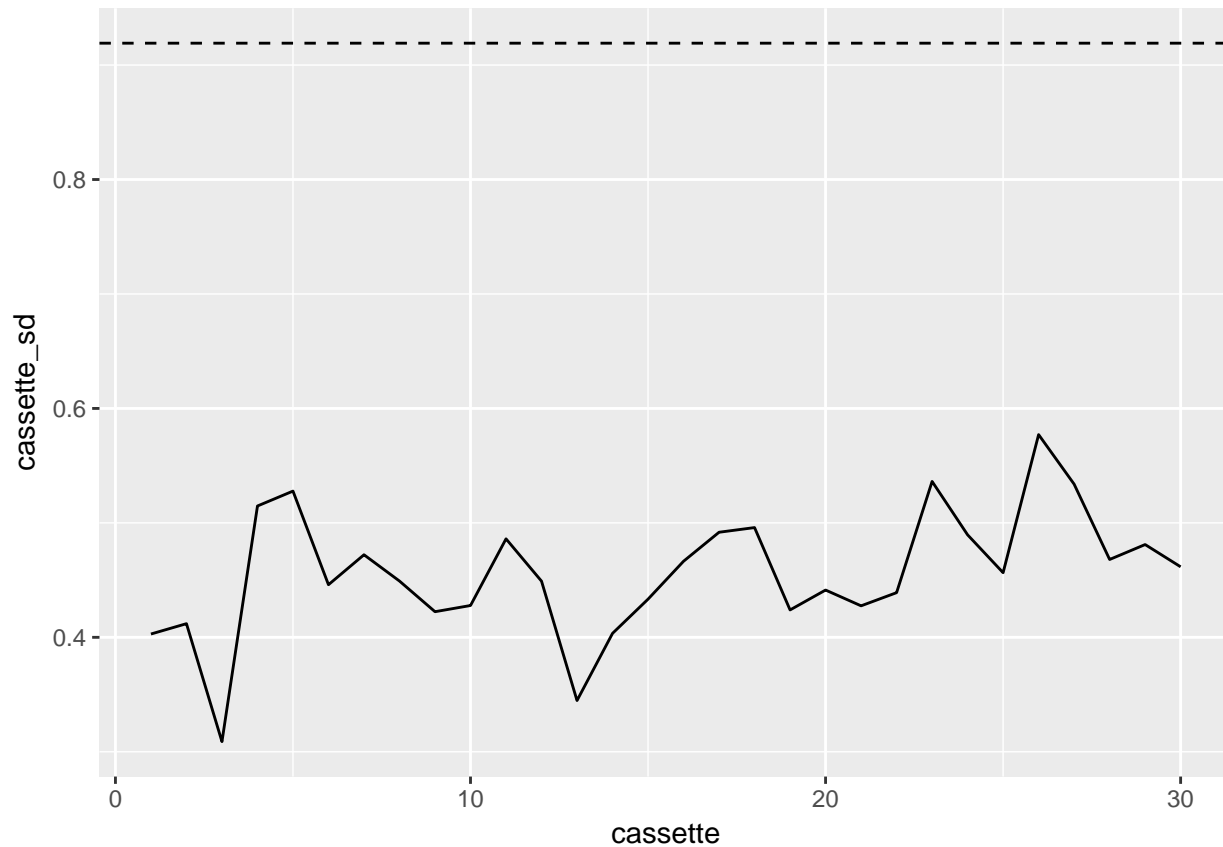
```
ggplot(litho_cassette) +
  geom_line(aes(cassette, cassette_mean)) +
  geom_hline(yintercept = mean_lw + 2*sd_lw/sqrt(15), linetype = "dashed") +
  geom_hline(yintercept = mean_lw - 2*sd_wafer/sqrt(15), linetype = "dashed") +
  geom_hline(yintercept = mean_lw)
```



#### 6.2.1.7.8 SD control chart by cassette

```
rms_sd_cassette <- litho_cassette %>%
  dplyr::select(cassette_sd) %>%
  mutate(sd_squared = cassette_sd^2) %$%
  sqrt(mean(sd_squared))

ggplot(litho_cassette) +
  geom_line(aes(cassette, cassette_sd)) +
  geom_hline(yintercept = 2*rms_sd_cassette, linetype = "dashed")
```



#### 6.2.1.7.9 Variance component estimation

Attach the necessary libraries

```
library(lme4)
library(broom)
```

Fit the random effects model and print the variance components

```
random_effects_model <- lmer(raw_linewidth ~ 1 | cassette/wafer, data = litho)
summary(random_effects_model)
```

```
## Linear mixed model fit by REML ['lmerMod']
## Formula: raw_linewidth ~ 1 | cassette/wafer
## Data: litho
##
## REML criterion at convergence: 645.5
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -2.45850 -0.62363 -0.03559  0.57612  2.52347
##
## Random effects:
## Groups       Name                Variance Std.Dev.
## wafer:cassette (Intercept) 0.04997  0.2235
## cassette      (Intercept) 0.26452  0.5143
## Residual                                0.17550  0.4189
## Number of obs: 450, groups: wafer:cassette, 90; cassette, 30
```

```
##
## Fixed effects:
##           Estimate Std. Error t value
## (Intercept)  2.53228    0.09881   25.63
```

```
augment(random_effects_model)
```

##	raw_linewidth	cassette	wafer	.fitted	.resid	.fixed	.mu
## 1	3.199275	1	1	2.397405	0.801869573	2.532284	2.397405
## 2	2.253081	1	1	2.397405	-0.144324427	2.532284	2.397405
## 3	2.074308	1	1	2.397405	-0.323097427	2.532284	2.397405
## 4	2.418206	1	1	2.397405	0.020800573	2.532284	2.397405
## 5	2.393732	1	1	2.397405	-0.003673427	2.532284	2.397405
## 6	2.654947	1	2	2.196917	0.458029715	2.532284	2.196917
## 7	2.003234	1	2	2.196917	-0.193683285	2.532284	2.196917
## 8	1.861268	1	2	2.196917	-0.335649285	2.532284	2.196917
## 9	2.136102	1	2	2.196917	-0.060815285	2.532284	2.196917
## 10	1.976495	1	2	2.196917	-0.220422285	2.532284	2.196917
## 11	2.887053	1	3	2.253183	0.633869650	2.532284	2.253183
## 12	2.061239	1	3	2.253183	-0.191944350	2.532284	2.253183
## 13	1.625191	1	3	2.253183	-0.627992350	2.532284	2.253183
## 14	2.304313	1	3	2.253183	0.051129650	2.532284	2.253183
## 15	2.233187	1	3	2.253183	-0.019996350	2.532284	2.253183
## 16	3.160233	2	1	2.318913	0.841320221	2.532284	2.318913
## 17	2.518913	2	1	2.318913	0.200000221	2.532284	2.318913
## 18	2.072211	2	1	2.318913	-0.246701779	2.532284	2.318913
## 19	2.287210	2	1	2.318913	-0.031702779	2.532284	2.318913
## 20	2.120452	2	1	2.318913	-0.198460779	2.532284	2.318913
## 21	2.063058	2	2	1.987554	0.075503944	2.532284	1.987554
## 22	2.217220	2	2	1.987554	0.229665944	2.532284	1.987554
## 23	1.472945	2	2	1.987554	-0.514609056	2.532284	1.987554
## 24	1.684581	2	2	1.987554	-0.302973056	2.532284	1.987554
## 25	1.900688	2	2	1.987554	-0.086866056	2.532284	1.987554
## 26	2.346254	2	3	2.097438	0.248816193	2.532284	2.097438
## 27	2.172825	2	3	2.097438	0.075387193	2.532284	2.097438
## 28	1.536538	2	3	2.097438	-0.560899807	2.532284	2.097438
## 29	1.966630	2	3	2.097438	-0.130807807	2.532284	2.097438
## 30	2.251576	2	3	2.097438	0.154138193	2.532284	2.097438
## 31	2.198141	3	1	1.733829	0.464312376	2.532284	1.733829
## 32	1.728784	3	1	1.733829	-0.005044624	2.532284	1.733829
## 33	1.357348	3	1	1.733829	-0.376480624	2.532284	1.733829
## 34	1.673159	3	1	1.733829	-0.060669624	2.532284	1.733829
## 35	1.429586	3	1	1.733829	-0.304242624	2.532284	1.733829
## 36	2.231291	3	2	1.824294	0.406997082	2.532284	1.824294
## 37	1.561993	3	2	1.824294	-0.262300918	2.532284	1.824294
## 38	1.520104	3	2	1.824294	-0.304189918	2.532284	1.824294
## 39	2.066068	3	2	1.824294	0.241774082	2.532284	1.824294
## 40	1.777603	3	2	1.824294	-0.046690918	2.532284	1.824294
## 41	2.244736	3	3	1.748700	0.496036378	2.532284	1.748700
## 42	1.745877	3	3	1.748700	-0.002822622	2.532284	1.748700
## 43	1.366895	3	3	1.748700	-0.381804622	2.532284	1.748700
## 44	1.615229	3	3	1.748700	-0.133470622	2.532284	1.748700
## 45	1.540863	3	3	1.748700	-0.207836622	2.532284	1.748700
## 46	2.929037	4	1	2.288878	0.640159073	2.532284	2.288878
## 47	2.035900	4	1	2.288878	-0.252977927	2.532284	2.288878

## 48	1.786147	4	1	2.288878	-0.502730927	2.532284	2.288878
## 49	1.980323	4	1	2.288878	-0.308554927	2.532284	2.288878
## 50	2.162919	4	1	2.288878	-0.125958927	2.532284	2.288878
## 51	2.855798	4	2	2.316285	0.539512663	2.532284	2.316285
## 52	2.104193	4	2	2.316285	-0.212092337	2.532284	2.316285
## 53	1.919507	4	2	2.316285	-0.396778337	2.532284	2.316285
## 54	2.019415	4	2	2.316285	-0.296870337	2.532284	2.316285
## 55	2.228705	4	2	2.316285	-0.087580337	2.532284	2.316285
## 56	3.219292	4	3	2.714948	0.504343818	2.532284	2.714948
## 57	2.900430	4	3	2.714948	0.185481818	2.532284	2.714948
## 58	2.171262	4	3	2.714948	-0.543686182	2.532284	2.714948
## 59	3.041250	4	3	2.714948	0.326301818	2.532284	2.714948
## 60	3.188804	4	3	2.714948	0.473855818	2.532284	2.714948
## 61	3.051234	5	1	2.702226	0.349007940	2.532284	2.702226
## 62	2.506230	5	1	2.702226	-0.195996060	2.532284	2.702226
## 63	1.950486	5	1	2.702226	-0.751740060	2.532284	2.702226
## 64	2.467719	5	1	2.702226	-0.234507060	2.532284	2.702226
## 65	2.581881	5	1	2.702226	-0.120345060	2.532284	2.702226
## 66	3.857221	5	2	3.140901	0.716319781	2.532284	3.140901
## 67	3.347343	5	2	3.140901	0.206441781	2.532284	3.140901
## 68	2.533870	5	2	3.140901	-0.607031219	2.532284	3.140901
## 69	3.190375	5	2	3.140901	0.049473781	2.532284	3.140901
## 70	3.362746	5	2	3.140901	0.221844781	2.532284	3.140901
## 71	3.690306	5	3	3.161507	0.528799176	2.532284	3.161507
## 72	3.401584	5	3	3.161507	0.240077176	2.532284	3.161507
## 73	2.963117	5	3	3.161507	-0.198389824	2.532284	3.161507
## 74	2.945828	5	3	3.161507	-0.215678824	2.532284	3.161507
## 75	3.466115	5	3	3.161507	0.304608176	2.532284	3.161507
## 76	2.938241	6	1	2.538503	0.399738314	2.532284	2.538503
## 77	2.526568	6	1	2.538503	-0.011934686	2.532284	2.538503
## 78	1.941370	6	1	2.538503	-0.597132686	2.532284	2.538503
## 79	2.765849	6	1	2.538503	0.227346314	2.532284	2.538503
## 80	2.382781	6	1	2.538503	-0.155721686	2.532284	2.538503
## 81	3.219665	6	2	2.572006	0.647658691	2.532284	2.572006
## 82	2.296011	6	2	2.572006	-0.275995309	2.532284	2.572006
## 83	2.256196	6	2	2.572006	-0.315810309	2.532284	2.572006
## 84	2.645933	6	2	2.572006	0.073926691	2.532284	2.572006
## 85	2.422187	6	2	2.572006	-0.149819309	2.532284	2.572006
## 86	3.180348	6	3	2.631210	0.549138363	2.532284	2.631210
## 87	2.849264	6	3	2.631210	0.218054363	2.532284	2.631210
## 88	1.601288	6	3	2.631210	-1.029921637	2.532284	2.631210
## 89	2.810051	6	3	2.631210	0.178841363	2.532284	2.631210
## 90	2.902980	6	3	2.631210	0.271770363	2.532284	2.631210
## 91	2.169679	7	1	2.123160	0.046518853	2.532284	2.123160
## 92	2.026506	7	1	2.123160	-0.096654147	2.532284	2.123160
## 93	1.671804	7	1	2.123160	-0.451356147	2.532284	2.123160
## 94	1.660760	7	1	2.123160	-0.462400147	2.532284	2.123160
## 95	2.314734	7	1	2.123160	0.191573853	2.532284	2.123160
## 96	2.912838	7	2	2.338686	0.574152360	2.532284	2.338686
## 97	2.323665	7	2	2.338686	-0.015020640	2.532284	2.338686
## 98	1.854223	7	2	2.338686	-0.484462640	2.532284	2.338686
## 99	2.391240	7	2	2.338686	0.052554360	2.532284	2.338686
## 100	2.196071	7	2	2.338686	-0.142614640	2.532284	2.338686
## 101	3.318517	7	3	2.531614	0.786902777	2.532284	2.531614

## 102	2.702735	7	3	2.531614	0.171120777	2.532284	2.531614
## 103	1.959008	7	3	2.531614	-0.572606223	2.532284	2.531614
## 104	2.512517	7	3	2.531614	-0.019097223	2.532284	2.531614
## 105	2.827469	7	3	2.531614	0.295854777	2.532284	2.531614
## 106	1.958022	8	1	1.689584	0.268438271	2.532284	1.689584
## 107	1.360106	8	1	1.689584	-0.329477729	2.532284	1.689584
## 108	0.971193	8	1	1.689584	-0.718390729	2.532284	1.689584
## 109	1.947857	8	1	1.689584	0.258273271	2.532284	1.689584
## 110	1.643580	8	1	1.689584	-0.046003729	2.532284	1.689584
## 111	2.357633	8	2	1.800398	0.557234600	2.532284	1.800398
## 112	1.757725	8	2	1.800398	-0.042673400	2.532284	1.800398
## 113	1.165886	8	2	1.800398	-0.634512400	2.532284	1.800398
## 114	2.231143	8	2	1.800398	0.430744600	2.532284	1.800398
## 115	1.311626	8	2	1.800398	-0.488772400	2.532284	1.800398
## 116	2.421686	8	3	1.934560	0.487126019	2.532284	1.934560
## 117	1.993855	8	3	1.934560	0.059295019	2.532284	1.934560
## 118	1.402543	8	3	1.934560	-0.532016981	2.532284	1.934560
## 119	2.008543	8	3	1.934560	0.073983019	2.532284	1.934560
## 120	2.139370	8	3	1.934560	0.204810019	2.532284	1.934560
## 121	2.190676	9	1	1.959423	0.231253427	2.532284	1.959423
## 122	2.287483	9	1	1.959423	0.328060427	2.532284	1.959423
## 123	1.698943	9	1	1.959423	-0.260479573	2.532284	1.959423
## 124	1.925731	9	1	1.959423	-0.033691573	2.532284	1.959423
## 125	2.057440	9	1	1.959423	0.098017427	2.532284	1.959423
## 126	2.353597	9	2	1.812932	0.540665183	2.532284	1.812932
## 127	1.796236	9	2	1.812932	-0.016695817	2.532284	1.812932
## 128	1.241040	9	2	1.812932	-0.571891817	2.532284	1.812932
## 129	1.677429	9	2	1.812932	-0.135502817	2.532284	1.812932
## 130	1.845041	9	2	1.812932	0.032109183	2.532284	1.812932
## 131	2.012669	9	3	1.667946	0.344723358	2.532284	1.667946
## 132	1.523769	9	3	1.667946	-0.144176642	2.532284	1.667946
## 133	0.790789	9	3	1.667946	-0.877156642	2.532284	1.667946
## 134	2.001942	9	3	1.667946	0.333996358	2.532284	1.667946
## 135	1.350051	9	3	1.667946	-0.317894642	2.532284	1.667946
## 136	2.825749	10	1	2.357094	0.468654771	2.532284	2.357094
## 137	2.502445	10	1	2.357094	0.145350771	2.532284	2.357094
## 138	1.938239	10	1	2.357094	-0.418855229	2.532284	2.357094
## 139	2.349497	10	1	2.357094	-0.007597229	2.532284	2.357094
## 140	2.310817	10	1	2.357094	-0.046277229	2.532284	2.357094
## 141	3.074576	10	2	2.218263	0.856312640	2.532284	2.218263
## 142	2.057821	10	2	2.218263	-0.160442360	2.532284	2.218263
## 143	1.793617	10	2	2.218263	-0.424646360	2.532284	2.218263
## 144	1.862251	10	2	2.218263	-0.356012360	2.532284	2.218263
## 145	1.956753	10	2	2.218263	-0.261510360	2.532284	2.218263
## 146	3.072840	10	3	2.334552	0.738288287	2.532284	2.334552
## 147	2.291035	10	3	2.334552	-0.043516713	2.532284	2.334552
## 148	1.873878	10	3	2.334552	-0.460673713	2.532284	2.334552
## 149	2.475640	10	3	2.334552	0.141088287	2.532284	2.334552
## 150	2.021472	10	3	2.334552	-0.313079713	2.532284	2.334552
## 151	3.228835	11	1	2.634201	0.594634324	2.532284	2.634201
## 152	2.719495	11	1	2.634201	0.085294324	2.532284	2.634201
## 153	2.207198	11	1	2.634201	-0.427002676	2.532284	2.634201
## 154	2.391608	11	1	2.634201	-0.242592676	2.532284	2.634201
## 155	2.525587	11	1	2.634201	-0.108613676	2.532284	2.634201



## 156	2.891103	11	2	2.533058	0.358044656	2.532284	2.533058
## 157	2.738007	11	2	2.533058	0.204948656	2.532284	2.533058
## 158	1.668337	11	2	2.533058	-0.864721344	2.532284	2.533058
## 159	2.496426	11	2	2.533058	-0.036632344	2.532284	2.533058
## 160	2.417926	11	2	2.533058	-0.115132344	2.532284	2.533058
## 161	3.541799	11	3	2.843834	0.697964510	2.532284	2.843834
## 162	3.058768	11	3	2.843834	0.214933510	2.532284	2.843834
## 163	2.187061	11	3	2.843834	-0.656773490	2.532284	2.843834
## 164	2.790261	11	3	2.843834	-0.053573490	2.532284	2.843834
## 165	3.279238	11	3	2.843834	0.435403510	2.532284	2.843834
## 166	2.347662	12	1	1.748642	0.599020267	2.532284	1.748642
## 167	1.383336	12	1	1.748642	-0.365305733	2.532284	1.748642
## 168	1.187168	12	1	1.748642	-0.561473733	2.532284	1.748642
## 169	1.693292	12	1	1.748642	-0.055349733	2.532284	1.748642
## 170	1.664072	12	1	1.748642	-0.084569733	2.532284	1.748642
## 171	2.385320	12	2	1.842730	0.542589503	2.532284	1.842730
## 172	1.607784	12	2	1.842730	-0.234946497	2.532284	1.842730
## 173	1.230307	12	2	1.842730	-0.612423497	2.532284	1.842730
## 174	1.945423	12	2	1.842730	0.102692503	2.532284	1.842730
## 175	1.907580	12	2	1.842730	0.064849503	2.532284	1.842730
## 176	2.691576	12	3	1.931171	0.760405467	2.532284	1.931171
## 177	1.938755	12	3	1.931171	0.007584467	2.532284	1.931171
## 178	1.275409	12	3	1.931171	-0.655761533	2.532284	1.931171
## 179	1.777315	12	3	1.931171	-0.153855533	2.532284	1.931171
## 180	2.146161	12	3	1.931171	0.214990467	2.532284	1.931171
## 181	3.218655	13	1	2.746640	0.472015127	2.532284	2.746640
## 182	2.912180	13	1	2.746640	0.165540127	2.532284	2.746640
## 183	2.336436	13	1	2.746640	-0.410203873	2.532284	2.746640
## 184	2.956036	13	1	2.746640	0.209396127	2.532284	2.746640
## 185	2.423235	13	1	2.746640	-0.323404873	2.532284	2.746640
## 186	3.302224	13	2	2.777867	0.524357171	2.532284	2.777867
## 187	2.808816	13	2	2.777867	0.030949171	2.532284	2.777867
## 188	2.340386	13	2	2.777867	-0.437480829	2.532284	2.777867
## 189	2.795120	13	2	2.777867	0.017253171	2.532284	2.777867
## 190	2.865800	13	2	2.777867	0.087933171	2.532284	2.777867
## 191	2.992217	13	3	2.652991	0.339226160	2.532284	2.652991
## 192	2.952106	13	3	2.652991	0.299115160	2.532284	2.652991
## 193	2.149299	13	3	2.652991	-0.503691840	2.532284	2.652991
## 194	2.448046	13	3	2.652991	-0.204944840	2.532284	2.652991
## 195	2.507733	13	3	2.652991	-0.145257840	2.532284	2.652991
## 196	3.530112	14	1	2.930121	0.599990877	2.532284	2.930121
## 197	2.940489	14	1	2.930121	0.010367877	2.532284	2.930121
## 198	2.598357	14	1	2.930121	-0.331764123	2.532284	2.930121
## 199	2.905165	14	1	2.930121	-0.024956123	2.532284	2.930121
## 200	2.692078	14	1	2.930121	-0.238043123	2.532284	2.930121
## 201	3.764270	14	2	3.045290	0.718980355	2.532284	3.045290
## 202	3.465960	14	2	3.045290	0.420670355	2.532284	3.045290
## 203	2.458628	14	2	3.045290	-0.586661645	2.532284	3.045290
## 204	3.141132	14	2	3.045290	0.095842355	2.532284	3.045290
## 205	2.816526	14	2	3.045290	-0.228763645	2.532284	3.045290
## 206	3.217614	14	3	2.875946	0.341667894	2.532284	2.875946
## 207	2.758171	14	3	2.875946	-0.117775106	2.532284	2.875946
## 208	2.345921	14	3	2.875946	-0.530025106	2.532284	2.875946
## 209	2.773653	14	3	2.875946	-0.102293106	2.532284	2.875946

## 210	3.109704	14	3	2.875946	0.233757894	2.532284	2.875946
## 211	2.177593	15	1	1.628454	0.549138745	2.532284	1.628454
## 212	1.511781	15	1	1.628454	-0.116673255	2.532284	1.628454
## 213	0.746546	15	1	1.628454	-0.881908255	2.532284	1.628454
## 214	1.491730	15	1	1.628454	-0.136724255	2.532284	1.628454
## 215	1.268580	15	1	1.628454	-0.359874255	2.532284	1.628454
## 216	2.433994	15	2	1.965194	0.468799916	2.532284	1.965194
## 217	2.045667	15	2	1.965194	0.080472916	2.532284	1.965194
## 218	1.612699	15	2	1.965194	-0.352495084	2.532284	1.965194
## 219	2.082860	15	2	1.965194	0.117665916	2.532284	1.965194
## 220	1.887341	15	2	1.965194	-0.077853084	2.532284	1.965194
## 221	1.923003	15	3	1.979982	-0.056978905	2.532284	1.979982
## 222	2.124461	15	3	1.979982	0.144479095	2.532284	1.979982
## 223	1.945048	15	3	1.979982	-0.034933905	2.532284	1.979982
## 224	2.210698	15	3	1.979982	0.230716095	2.532284	1.979982
## 225	1.985225	15	3	1.979982	0.005243095	2.532284	1.979982
## 226	3.131536	16	1	2.585214	0.546321560	2.532284	2.585214
## 227	2.405975	16	1	2.585214	-0.179239440	2.532284	2.585214
## 228	2.206320	16	1	2.585214	-0.378894440	2.532284	2.585214
## 229	3.012211	16	1	2.585214	0.426996560	2.532284	2.585214
## 230	2.628723	16	1	2.585214	0.043508560	2.532284	2.585214
## 231	2.802486	16	2	2.330170	0.472315945	2.532284	2.330170
## 232	2.185010	16	2	2.330170	-0.145160055	2.532284	2.330170
## 233	2.161802	16	2	2.330170	-0.168368055	2.532284	2.330170
## 234	2.102560	16	2	2.330170	-0.227610055	2.532284	2.330170
## 235	1.961968	16	2	2.330170	-0.368202055	2.532284	2.330170
## 236	3.330183	16	3	2.433764	0.896419252	2.532284	2.433764
## 237	2.464046	16	3	2.433764	0.030282252	2.532284	2.433764
## 238	1.687408	16	3	2.433764	-0.746355748	2.532284	2.433764
## 239	2.043322	16	3	2.433764	-0.390441748	2.532284	2.433764
## 240	2.570657	16	3	2.433764	0.136893252	2.532284	2.433764
## 241	3.352633	17	1	2.460815	0.891817709	2.532284	2.460815
## 242	2.691645	17	1	2.460815	0.230829709	2.532284	2.460815
## 243	1.942410	17	1	2.460815	-0.518405291	2.532284	2.460815
## 244	2.366055	17	1	2.460815	-0.094760291	2.532284	2.460815
## 245	2.500987	17	1	2.460815	0.040171709	2.532284	2.460815
## 246	2.886284	17	2	2.279169	0.607114639	2.532284	2.279169
## 247	2.292503	17	2	2.279169	0.013333639	2.532284	2.279169
## 248	1.627562	17	2	2.279169	-0.651607361	2.532284	2.279169
## 249	2.415076	17	2	2.279169	0.135906639	2.532284	2.279169
## 250	2.086134	17	2	2.279169	-0.193035361	2.532284	2.279169
## 251	2.554848	17	3	2.129874	0.424974257	2.532284	2.129874
## 252	1.755843	17	3	2.129874	-0.374030743	2.532284	2.129874
## 253	1.510124	17	3	2.129874	-0.619749743	2.532284	2.129874
## 254	2.257347	17	3	2.129874	0.127473257	2.532284	2.129874
## 255	1.958592	17	3	2.129874	-0.171281743	2.532284	2.129874
## 256	2.622733	18	1	2.191171	0.431561594	2.532284	2.191171
## 257	2.321079	18	1	2.191171	0.129907594	2.532284	2.191171
## 258	1.169269	18	1	2.191171	-1.021902406	2.532284	2.191171
## 259	1.921457	18	1	2.191171	-0.269714406	2.532284	2.191171
## 260	2.176377	18	1	2.191171	-0.014794406	2.532284	2.191171
## 261	3.313367	18	2	2.544520	0.768846869	2.532284	2.544520
## 262	2.559725	18	2	2.544520	0.015204869	2.532284	2.544520
## 263	2.404662	18	2	2.544520	-0.139858131	2.532284	2.544520

## 264	2.405249	18	2	2.544520	-0.139271131	2.532284	2.544520
## 265	2.535618	18	2	2.544520	-0.008902131	2.532284	2.544520
## 266	3.067851	18	3	2.449793	0.618058143	2.532284	2.449793
## 267	2.490359	18	3	2.449793	0.040566143	2.532284	2.449793
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## 269	2.669512	18	3	2.449793	0.219719143	2.532284	2.449793
## 270	2.105103	18	3	2.449793	-0.344689857	2.532284	2.449793
## 271	4.293889	19	1	3.531144	0.762745066	2.532284	3.531144
## 272	3.888826	19	1	3.531144	0.357682066	2.532284	3.531144
## 273	2.960655	19	1	3.531144	-0.570488934	2.532284	3.531144
## 274	3.618864	19	1	3.531144	0.087720066	2.532284	3.531144
## 275	3.562480	19	1	3.531144	0.031336066	2.532284	3.531144
## 276	3.451872	19	2	3.184155	0.267717185	2.532284	3.184155
## 277	3.285934	19	2	3.184155	0.101779185	2.532284	3.184155
## 278	2.638294	19	2	3.184155	-0.545860815	2.532284	3.184155
## 279	2.918810	19	2	3.184155	-0.265344815	2.532284	3.184155
## 280	3.076231	19	2	3.184155	-0.107923815	2.532284	3.184155
## 281	3.879683	19	3	3.459376	0.420306531	2.532284	3.459376
## 282	3.342026	19	3	3.459376	-0.117350469	2.532284	3.459376
## 283	3.382833	19	3	3.459376	-0.076543469	2.532284	3.459376
## 284	3.491666	19	3	3.459376	0.032289531	2.532284	3.459376
## 285	3.617621	19	3	3.459376	0.158244531	2.532284	3.459376
## 286	2.329987	20	1	2.375244	-0.045257340	2.532284	2.375244
## 287	2.400277	20	1	2.375244	0.025032660	2.532284	2.375244
## 288	2.033941	20	1	2.375244	-0.341303340	2.532284	2.375244
## 289	2.544367	20	1	2.375244	0.169122660	2.532284	2.375244
## 290	2.493079	20	1	2.375244	0.117834660	2.532284	2.375244
## 291	2.862084	20	2	2.359172	0.502911902	2.532284	2.359172
## 292	2.404703	20	2	2.359172	0.045530902	2.532284	2.359172
## 293	1.648662	20	2	2.359172	-0.710510098	2.532284	2.359172
## 294	2.115465	20	2	2.359172	-0.243707098	2.532284	2.359172
## 295	2.633930	20	2	2.359172	0.274757902	2.532284	2.359172
## 296	3.305211	20	3	2.429361	0.875850030	2.532284	2.429361
## 297	2.194991	20	3	2.429361	-0.234369970	2.532284	2.429361
## 298	1.620963	20	3	2.429361	-0.808397970	2.532284	2.429361
## 299	2.322678	20	3	2.429361	-0.106682970	2.532284	2.429361
## 300	2.818449	20	3	2.429361	0.389088030	2.532284	2.429361
## 301	2.712915	21	1	2.100673	0.612241684	2.532284	2.100673
## 302	2.389121	21	1	2.100673	0.288447684	2.532284	2.100673
## 303	1.575833	21	1	2.100673	-0.524840316	2.532284	2.100673
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## 305	2.203262	21	1	2.100673	0.102588684	2.532284	2.100673
## 306	2.607972	21	2	1.958099	0.649873442	2.532284	1.958099
## 307	2.177747	21	2	1.958099	0.219648442	2.532284	1.958099
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## 310	1.843187	21	2	1.958099	-0.114911558	2.532284	1.958099
## 311	2.277813	21	3	1.936304	0.341509308	2.532284	1.936304
## 312	1.764940	21	3	1.936304	-0.171363692	2.532284	1.936304
## 313	1.358137	21	3	1.936304	-0.578166692	2.532284	1.936304
## 314	2.065713	21	3	1.936304	0.129409308	2.532284	1.936304
## 315	1.885897	21	3	1.936304	-0.050406692	2.532284	1.936304
## 316	3.126184	22	1	2.613089	0.513095276	2.532284	2.613089
## 317	2.843505	22	1	2.613089	0.230416276	2.532284	2.613089

## 318	2.041466	22	1	2.613089	-0.571622724	2.532284	2.613089
## 319	2.816967	22	1	2.613089	0.203878276	2.532284	2.613089
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## 321	3.049442	22	2	2.459297	0.590145132	2.532284	2.459297
## 322	2.446904	22	2	2.459297	-0.012392868	2.532284	2.459297
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## 324	2.676519	22	2	2.459297	0.217222132	2.532284	2.459297
## 325	2.187865	22	2	2.459297	-0.271431868	2.532284	2.459297
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## 328	1.580387	22	3	2.420937	-0.840550044	2.532284	2.420937
## 329	2.508542	22	3	2.420937	0.087604956	2.532284	2.420937
## 330	2.574564	22	3	2.420937	0.153626956	2.532284	2.420937
## 331	3.294288	23	1	2.764077	0.530211208	2.532284	2.764077
## 332	2.641762	23	1	2.764077	-0.122314792	2.532284	2.764077
## 333	2.105774	23	1	2.764077	-0.658302792	2.532284	2.764077
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## 335	2.622482	23	1	2.764077	-0.141594792	2.532284	2.764077
## 336	4.066631	23	2	3.229016	0.837615083	2.532284	3.229016
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## 344	2.517418	23	3	2.797817	-0.280398553	2.532284	2.797817
## 345	2.862723	23	3	2.797817	0.064906447	2.532284	2.797817
## 346	4.212664	24	1	3.155523	1.057140501	2.532284	3.155523
## 347	3.068342	24	1	3.155523	-0.087181499	2.532284	3.155523
## 348	2.872188	24	1	3.155523	-0.283335499	2.532284	3.155523
## 349	3.040890	24	1	3.155523	-0.114633499	2.532284	3.155523
## 350	3.376318	24	1	3.155523	0.220794501	2.532284	3.155523
## 351	3.223384	24	2	2.847300	0.376084016	2.532284	2.847300
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## 356	3.359505	24	3	2.861631	0.497873609	2.532284	2.861631
## 357	2.800742	24	3	2.861631	-0.060889391	2.532284	2.861631
## 358	2.043396	24	3	2.861631	-0.818235391	2.532284	2.861631
## 359	2.929792	24	3	2.861631	0.068160609	2.532284	2.861631
## 360	2.935356	24	3	2.861631	0.073724609	2.532284	2.861631
## 361	2.724871	25	1	2.440734	0.284136829	2.532284	2.440734
## 362	2.239013	25	1	2.440734	-0.201721171	2.532284	2.440734
## 363	2.341512	25	1	2.440734	-0.099222171	2.532284	2.440734
## 364	2.263617	25	1	2.440734	-0.177117171	2.532284	2.440734
## 365	2.062748	25	1	2.440734	-0.377986171	2.532284	2.440734
## 366	3.658082	25	2	2.822441	0.835641036	2.532284	2.822441
## 367	3.093268	25	2	2.822441	0.270827036	2.532284	2.822441
## 368	2.429341	25	2	2.822441	-0.393099964	2.532284	2.822441
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## 370	3.161795	25	2	2.822441	0.339354036	2.532284	2.822441
## 371	3.178246	25	3	2.561028	0.617217839	2.532284	2.561028

## 372	2.498102	25	3	2.561028	-0.062926161	2.532284	2.561028
## 373	2.445810	25	3	2.561028	-0.115218161	2.532284	2.561028
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## 375	2.302298	25	3	2.561028	-0.258730161	2.532284	2.561028
## 376	3.320688	26	1	2.885606	0.435081630	2.532284	2.885606
## 377	2.861800	26	1	2.885606	-0.023806370	2.532284	2.885606
## 378	2.238258	26	1	2.885606	-0.647348370	2.532284	2.885606
## 379	3.122050	26	1	2.885606	0.236443630	2.532284	2.885606
## 380	3.160876	26	1	2.885606	0.275269630	2.532284	2.885606
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## 384	3.309867	26	2	3.101135	0.208732435	2.532284	3.101135
## 385	3.542882	26	2	3.101135	0.441747435	2.532284	3.101135
## 386	2.586453	26	3	2.486541	0.099911614	2.532284	2.486541
## 387	2.120604	26	3	2.486541	-0.365937386	2.532284	2.486541
## 388	2.180847	26	3	2.486541	-0.305694386	2.532284	2.486541
## 389	2.480888	26	3	2.486541	-0.005653386	2.532284	2.486541
## 390	1.938037	26	3	2.486541	-0.548504386	2.532284	2.486541
## 391	4.710718	27	1	4.073210	0.637507673	2.532284	4.073210
## 392	4.082083	27	1	4.073210	0.008872673	2.532284	4.073210
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## 401	5.168668	27	3	4.303624	0.865043796	2.532284	4.303624
## 402	4.823275	27	3	4.303624	0.519650796	2.532284	4.303624
## 403	3.764272	27	3	4.303624	-0.539352204	2.532284	4.303624
## 404	4.396897	27	3	4.303624	0.093272796	2.532284	4.303624
## 405	4.442094	27	3	4.303624	0.138469796	2.532284	4.303624
## 406	3.972279	28	1	3.405434	0.566845014	2.532284	3.405434
## 407	3.883295	28	1	3.405434	0.477861014	2.532284	3.405434
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## 409	3.514590	28	1	3.405434	0.109156014	2.532284	3.405434
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## 414	2.927978	28	2	2.966293	-0.038314662	2.532284	2.966293
## 415	3.152570	28	2	2.966293	0.186277338	2.532284	2.966293
## 416	3.558060	28	3	3.134582	0.423477722	2.532284	3.134582
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## 419	3.026064	28	3	3.134582	-0.108518278	2.532284	3.134582
## 420	3.071975	28	3	3.134582	-0.062607278	2.532284	3.134582
## 421	3.496634	29	1	2.797622	0.699011772	2.532284	2.797622
## 422	3.087091	29	1	2.797622	0.289468772	2.532284	2.797622
## 423	2.517673	29	1	2.797622	-0.279949228	2.532284	2.797622
## 424	2.547344	29	1	2.797622	-0.250278228	2.532284	2.797622
## 425	2.971948	29	1	2.797622	0.174325772	2.532284	2.797622

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## 437      2.695163      30      1 2.610508  0.084655464 2.532284 2.610508
## 438      2.229518      30      1 2.610508 -0.380989536 2.532284 2.610508
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## 441      3.537562      30      2 3.112203  0.425359367 2.532284 3.112203
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## 446      3.184652      30      3 2.827247  0.357405038 2.532284 2.827247
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## 2          0          1          1          1 -0.144324427
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## 406	0	1	1	1 0.566845014

```

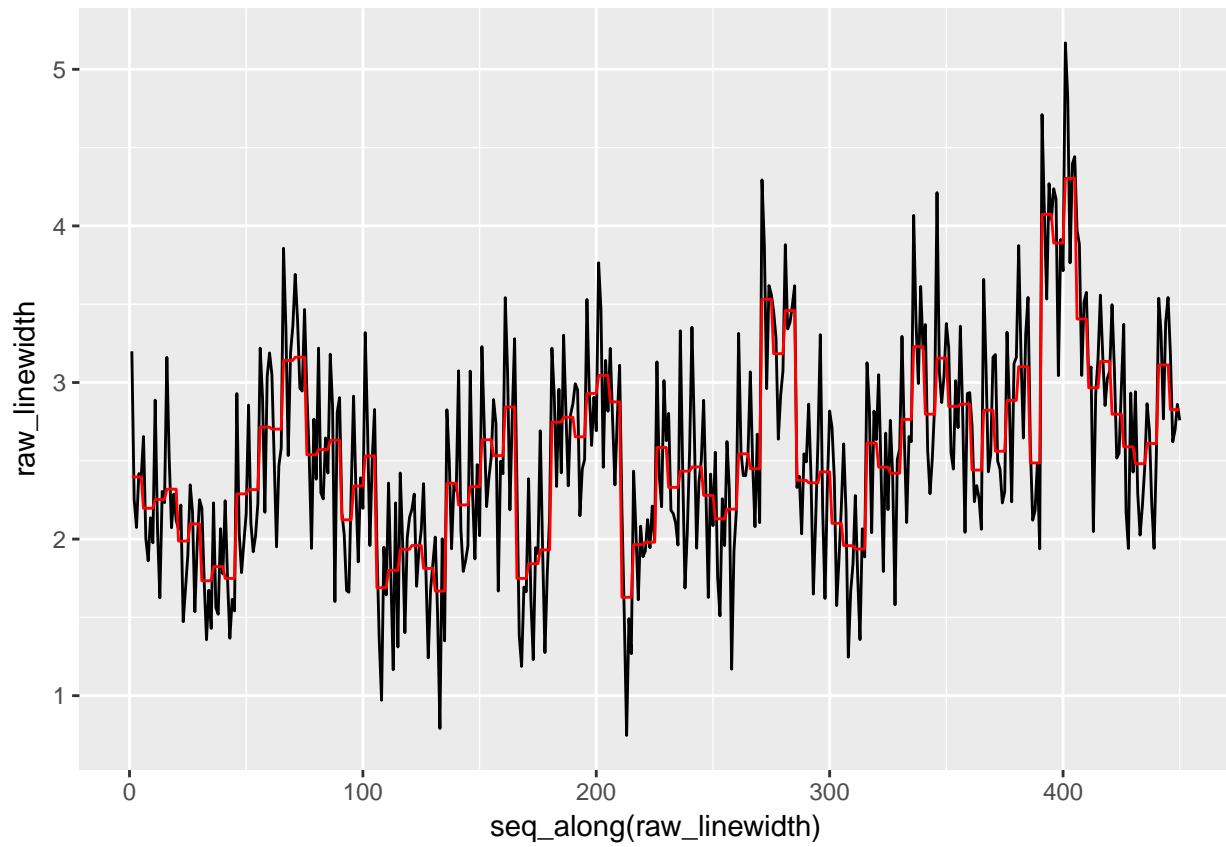
## 407      0      1      1      1  0.477861014
## 408      0      1      1      1 -0.360288986
## 409      0      1      1      1  0.109156014
## 410      0      1      1      1  0.170012014
## 411      0      1      1      1  0.058610338
## 412      0      1      1      1  0.132899338
## 413      0      1      1      1 -0.918153662
## 414      0      1      1      1 -0.038314662
## 415      0      1      1      1  0.186277338
## 416      0      1      1      1  0.423477722
## 417      0      1      1      1  0.041709722
## 418      0      1      1      1 -0.281709278
## 419      0      1      1      1 -0.108518278
## 420      0      1      1      1 -0.062607278
## 421      0      1      1      1  0.699011772
## 422      0      1      1      1  0.289468772
## 423      0      1      1      1 -0.279949228
## 424      0      1      1      1 -0.250278228
## 425      0      1      1      1  0.174325772
## 426      0      1      1      1  0.782065942
## 427      0      1      1      1 -0.414194058
## 428      0      1      1      1 -0.649129058
## 429      0      1      1      1  0.343167942
## 430      0      1      1      1 -0.161171058
## 431      0      1      1      1  0.459295244
## 432      0      1      1      1 -0.187736756
## 433      0      1      1      1 -0.456071756
## 434      0      1      1      1 -0.270205756
## 435      0      1      1      1 -0.022061756
## 436      0      1      1      1  0.254162464
## 437      0      1      1      1  0.084655464
## 438      0      1      1      1 -0.380989536
## 439      0      1      1      1 -0.669590536
## 440      0      1      1      1 -0.063189536
## 441      0      1      1      1  0.425359367
## 442      0      1      1      1  0.199158367
## 443      0      1      1      1 -0.344431633
## 444      0      1      1      1  0.276419367
## 445      0      1      1      1  0.430498367
## 446      0      1      1      1  0.357405038
## 447      0      1      1      1 -0.206299962
## 448      0      1      1      1 -0.129627962
## 449      0      1      1      1  0.033437038
## 450      0      1      1      1 -0.068675962

```

```

ggplot(augment(random_effects_model)) +
  geom_line(aes(seq_along(raw_linewidth), raw_linewidth)) +
  geom_line(aes(seq_along(raw_linewidth), .fitted), colour = "red")

```







## Chapter 7

# Product and Process Comparisons

### 7.1 Packages used in this chapter

```
library(magrittr) # used for %$% pipe
library(tidyverse)
library(ggplot2)
```

### 7.2 Exercises

#### 7.2.1 7.2.2. Are the data consistent with the assumed process mean?

process comparison

### 7.3 Student's t-test

#### 7.3.1 “illustrative example of the t-test” in section 7.2.2 - particle (contamination) counts

Over a long run the process average for wafer particle counts has been 50 counts per wafer. We want to test whether a change has occurred based on new data. The null hypothesis that the process mean is 50 counts is tested against the alternative hypothesis that the process mean is not equal to 50 counts.

$$H_0 : \mu = \mu_0$$

$$H_a : \mu \neq \mu_0$$

The purpose of the two-sided alternative is to rule out a possible process change in either direction.

```
particles <- tribble( ~test1, 50, 48, 44, 56, 61, 52, 53, 55, 67, 51)
particles
```

```
## # A tibble: 10 x 1
##   test1
##   <dbl>
```

```
## 1 50.
## 2 48.
## 3 44.
## 4 56.
## 5 61.
## 6 52.
## 7 53.
## 8 55.
## 9 67.
## 10 51.
```

We can generate the needed summary statistics:

```
particle_summary <- particles %>%
  summarise(particle_mean = mean(test1), particle_sd = sd(test1), particle_count = n())

particle_summary
```

```
## # A tibble: 1 x 3
##   particle_mean particle_sd particle_count
##         <dbl>         <dbl>         <int>
## 1         53.7         6.57             10
```

Let do this simple example by hand and then compare the result to the `t.test()` function from the `stats` package

$$t = \frac{\bar{Y} - \mu_0}{s \sqrt{n}}$$

```
t_particle <- (particle_summary$particle_mean - 50)/(particle_summary$particle_sd/sqrt(particle_summary$particle_count))
t_critical <- qt(1-0.05/2, df = particle_summary$particle_count - 1)
t_critical
```

```
## [1] 2.262157
```

```
t_particle
```

```
## [1] 1.781768
```

Because the value of `t_particle` is inside the interval  $(-2.26, 2.26)$ , we can not reject the null hypothesis and, therefore, we may continue to assume the process mean is 50 counts.

```
particle_summary_t <- particles %>%
  summarise(particle_mean = mean(test1), particle_sd = sd(test1), particle_count = n(), t_particle = (particle_mean - 50)/(particle_sd/sqrt(particle_count)), t_critical = qt(1-0.05/2, df = particle_count - 1))

particle_summary_t
```

```
## # A tibble: 1 x 5
##   particle_mean particle_sd particle_count t_particle t_critical
##         <dbl>         <dbl>         <int>         <dbl>         <dbl>
## 1         53.7         6.57             10         1.78         2.26
```

An alternative method would be to use the `t.test()` function

```
particle_t_test <- t.test(particles$test1, alternative = "two.sided", mu = 50, conf.level = 0.95)
particle_t_test
```

```
##
## One Sample t-test
```

```
##
## data:  particles$test1
## t = 1.7818, df = 9, p-value = 0.1085
## alternative hypothesis: true mean is not equal to 50
## 95 percent confidence interval:
##  49.00243 58.39757
## sample estimates:
## mean of x
##      53.7
```

#### NEW function alert!

Load the library(magrittr) to use the %\$% function. This allows calling column names within the piped function which is useful for working with base R functions

```
# library(magrittr) # to use the %$% function; allows calling column names within the piped function; u

particle_t_test2 <- particles %$%
  t.test(test1, alternative = "two.sided", mu = 50, conf.level = 0.95)
particle_t_test2
```

```
##
## One Sample t-test
##
## data:  test1
## t = 1.7818, df = 9, p-value = 0.1085
## alternative hypothesis: true mean is not equal to 50
## 95 percent confidence interval:
##  49.00243 58.39757
## sample estimates:
## mean of x
##      53.7
```

### 7.3.2 Do two processes have the same mean? in section 7.3.1 - Example of unequal number of data points

A new procedure (process 2) to assemble a device is introduced and tested for possible improvement in time of assembly. The question being addressed is whether the mean, 2, of the new assembly process is smaller than the mean, 1, for the old assembly process (process 1).

$$H_0 : \mu_{process\ 2} = \mu_{process\ 1}$$

$$H_a : \mu_{process\ 2} < \mu_{process\ 1}$$

```
device_test <- tribble(
  ~device, ~process_old, ~process_new,
  1, 32, 36,
  2, 37, 31,
  3, 35, 30,
  4, 28, 31,
  5, 41, 34,
  6, 44, 36,
  7, 35, 29,
  8, 31, 32,
  9, 34, 31,
  10, 38, NA,
```

```
11, 42, NA)
```

```
device_test
```

```
## # A tibble: 11 x 3
##   device process_old process_new
##   <dbl>      <dbl>      <dbl>
## 1     1.        32.        36.
## 2     2.        37.        31.
## 3     3.        35.        30.
## 4     4.        28.        31.
## 5     5.        41.        34.
## 6     6.        44.        36.
## 7     7.        35.        29.
## 8     8.        31.        32.
## 9     9.        34.        31.
## 10    10.        38.        NA
## 11    11.        42.        NA
```

```
device_summary <- device_test %>%
  dplyr::select(process_old, process_new) %>%
  summary()
```

```
device_summary
```

```
##   process_old    process_new
##   Min.   :28.00   Min.   :29.00
##   1st Qu.:33.00   1st Qu.:31.00
##   Median :35.00   Median :31.00
##   Mean   :36.09   Mean   :32.22
##   3rd Qu.:39.50   3rd Qu.:34.00
##   Max.   :44.00   Max.   :36.00
##               NA's   :2
```

```
device_t_test <- device_test %$%
  t.test(process_new, process_old, alternative = "less", var.equal = FALSE, conf.level = 0.95)
device_t_test
```

```
##
## Welch Two Sample t-test
##
## data: process_new and process_old
## t = -2.2694, df = 15.533, p-value = 0.01894
## alternative hypothesis: true difference in means is less than 0
## 95 percent confidence interval:
##      -Inf -0.8869087
## sample estimates:
## mean of x mean of y
## 32.22222 36.09091
## (-qt(1-0.05, df = 15.533))
```

```
## [1] -1.749109
```

## 7.4 One more classic example! (from Student himself)

From the article

I will conclude with an example which comes beyond the range of the tables, there being eleven experiments.

To test whether it is of advantage to kiln-dry barley seed before sowing, seven varieties of barley were sown (both kiln-dried and not kiln-dried in 1899 and four in 1900; the results are given in the table.

```
corn <- read_table2("sample reg kiln
1 1903 2009
2 1935 1915
3 1910 2011
4 2496 2463
5 2108 2180
6 1961 1925
7 2060 2122
8 1444 1482
9 1612 1542
10 1316 1443
11 1511 1535", col_names = TRUE, col_types = cols("i", "d", "d"))

corn %<>% mutate(year = case_when(
  sample <= 7 ~ "cy1889",
  sample > 7 ~ "cy1900"
))

corn

## # A tibble: 11 x 4
##   sample  reg  kiln year
##   <int> <dbl> <dbl> <chr>
## 1     1 1903. 2009. cy1889
## 2     2 1935. 1915. cy1889
## 3     3 1910. 2011. cy1889
## 4     4 2496. 2463. cy1889
## 5     5 2108. 2180. cy1889
## 6     6 1961. 1925. cy1889
## 7     7 2060. 2122. cy1889
## 8     8 1444. 1482. cy1900
## 9     9 1612. 1542. cy1900
## 10    10 1316. 1443. cy1900
## 11    11 1511. 1535. cy1900

corn_t_test_wrong <- corn %$%
  t.test(reg, kiln, alternative = "two.sided", var.equal = TRUE, conf.level = 0.95)

corn_t_test_wrong

##
## Two Sample t-test
##
## data:  reg and kiln
## t = -0.23413, df = 20, p-value = 0.8173
```

```
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -334.2127 266.7581
## sample estimates:
## mean of x mean of y
## 1841.455 1875.182

corn_t_test_correct <- corn %$%
  t.test(reg, kiln, paired = TRUE, alternative = "two.sided", var.equal = TRUE, conf.level = 0.95)

corn_t_test_correct

##
## Paired t-test
##
## data: reg and kiln
## t = -1.6905, df = 10, p-value = 0.1218
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
## -78.18164 10.72710
## sample estimates:
## mean of the differences
## -33.72727
```

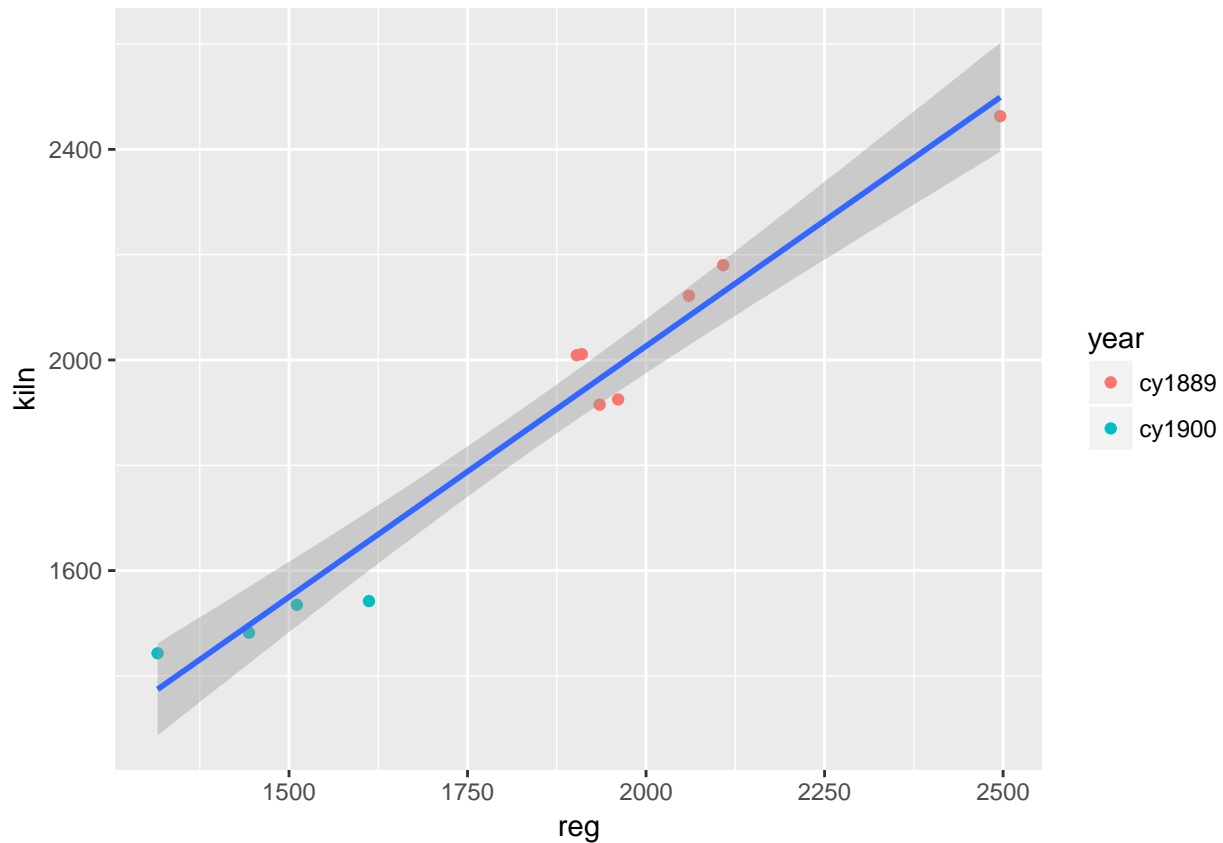
#### 7.4.1 plot of Student's (W.S. Gossett) data

```
corn_tidy <- corn %>%
  gather(reg, kiln, key = treatment, value = "yield")

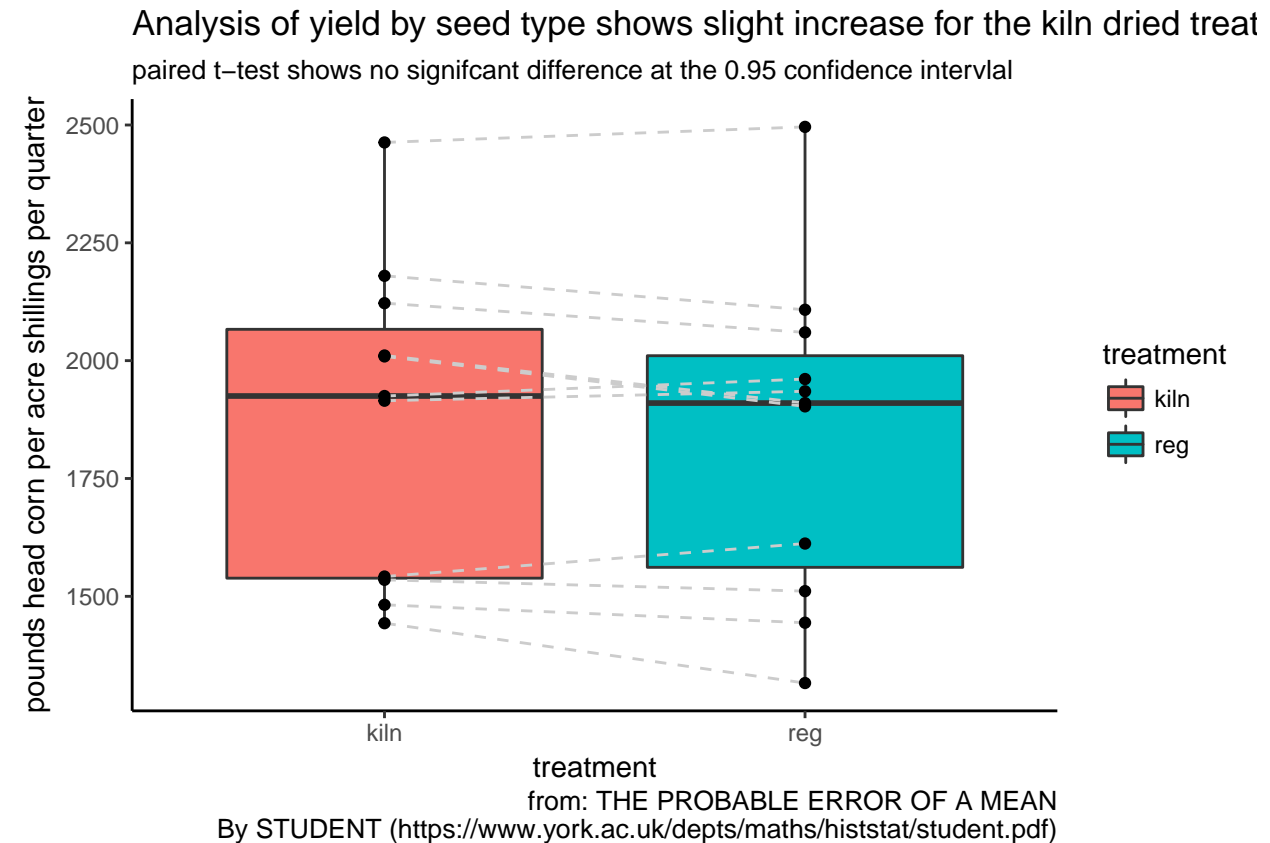
corn_tidy
```

```
## # A tibble: 22 x 4
##   sample year treatment yield
##   <int> <chr> <chr> <dbl>
## 1     1 1 cy1889 reg      1903.
## 2     2 2 cy1889 reg      1935.
## 3     3 3 cy1889 reg      1910.
## 4     4 4 cy1889 reg      2496.
## 5     5 5 cy1889 reg      2108.
## 6     6 6 cy1889 reg      1961.
## 7     7 7 cy1889 reg      2060.
## 8     8 8 cy1900 reg      1444.
## 9     9 9 cy1900 reg      1612.
## 10    10 10 cy1900 reg      1316.
## # ... with 12 more rows
```

```
ggplot(corn) +
  geom_point(aes(reg, kiln, colour = year)) +
  geom_smooth(aes(reg, kiln), method = "lm")
```



```
ggplot(corn_tidy, aes(treatment, yield)) +
  geom_boxplot(aes(fill = treatment)) +
  geom_line(aes(group = sample), linetype = "dashed", colour = "grey80") +
  geom_point() +
  theme_classic() +
  labs(title = "Analysis of yield by seed type shows slight increase for the kiln dried treatement",
        subtitle = "paired t-test shows no significant difference at the 0.95 confidence intervla",
        y = "pounds head corn per acre shillings per quarter", caption = "from: THE PROBABLE ERROR OF A I
By STUDENT (https://www.york.ac.uk/depts/math/histstat/student.pdf)")
```



## 7.5 Anova

From the *NIST Engineering and Statistics Handbook*

ANOVA is a general technique that can be used to test the hypothesis that the means among two or more groups are equal, under the assumption that the sampled populations are normally distributed.

The ANOVA procedure is one of the most powerful statistical techniques

The following example is adapted from <https://onlinecourses.science.psu.edu/stat502/node/150>

a plant biologist thinks that plant height may be affected by applying different fertilizers. They tested three kinds of fertilizer and also one group of plants that are untreated (the control). They kept all the plants under controlled conditions in the greenhouse. (In addition, we need to have some information about replication and randomization.) They randomly assigned the fertilizer treatment levels to individual containerized plants to produce 6 replications of each of the fertilizer applications.

Image available

```
lesson1_data <- read_table2("Control  F1  F2  F3
21  32  22.5  28
19.5  30.5  26  27.5
22.5  25  28  31
21.5  27.5  27  29.5
20.5  28  26.5  30")
```



```
21 28.6 25.2 29.2", col_names = TRUE)
lesson1_data
```

```
## # A tibble: 6 x 4
##   Control    F1    F2    F3
##   <dbl> <dbl> <dbl> <dbl>
## 1  21.0  32.0  22.5  28.0
## 2  19.5  30.5  26.0  27.5
## 3  22.5  25.0  28.0  31.0
## 4  21.5  27.5  27.0  29.5
## 5  20.5  28.0  26.5  30.0
## 6  21.0  28.6  25.2  29.2
```

### One-way ANOVA table: the basic format

Source of Variation	Sum of Squares (SS)	Degrees of Freedom (df)	Mean Squares (MS)	F-Ratio
Between samples	SSB	k - 1	MSB	MSB/MSW
Within samples	SSW	n(total) - k	MSW	
<i>Total</i>	SST	n(total) - 1		

### One-way ANOVA table: NIST Handbook

Source	SS	DF	MS	F
Treatments	SST	k-1	SST/(k-1)	MST/MSE
Error	SSE	N-k	SSE/(N-k)	
<i>Total (corrected)</i>	SS	N-1		

$$\text{Total Sum of Squares } SST = \sum_{i=1}^k \sum_{j=1}^{n_i} (x_{ij} - \bar{\bar{x}})^2$$

#### 7.5.1 Tidy the data and compute the sum of squares

```
lesson1_gather <- lesson1_data %>%
  gather(key = treatment, value = value, Control, F1, F2, F3)
lesson1_gather
```

```
## # A tibble: 24 x 2
##   treatment value
##   <chr>      <dbl>
## 1 Control    21.0
## 2 Control    19.5
## 3 Control    22.5
## 4 Control    21.5
## 5 Control    20.5
## 6 Control    21.0
## 7 F1        32.0
## 8 F1        30.5
## 9 F1        25.0
```

```
## 10 F1          27.5
## # ... with 14 more rows

lesson1_grand_mean <- lesson1_gather %>%
  mean(value)

lesson1_grand_mean

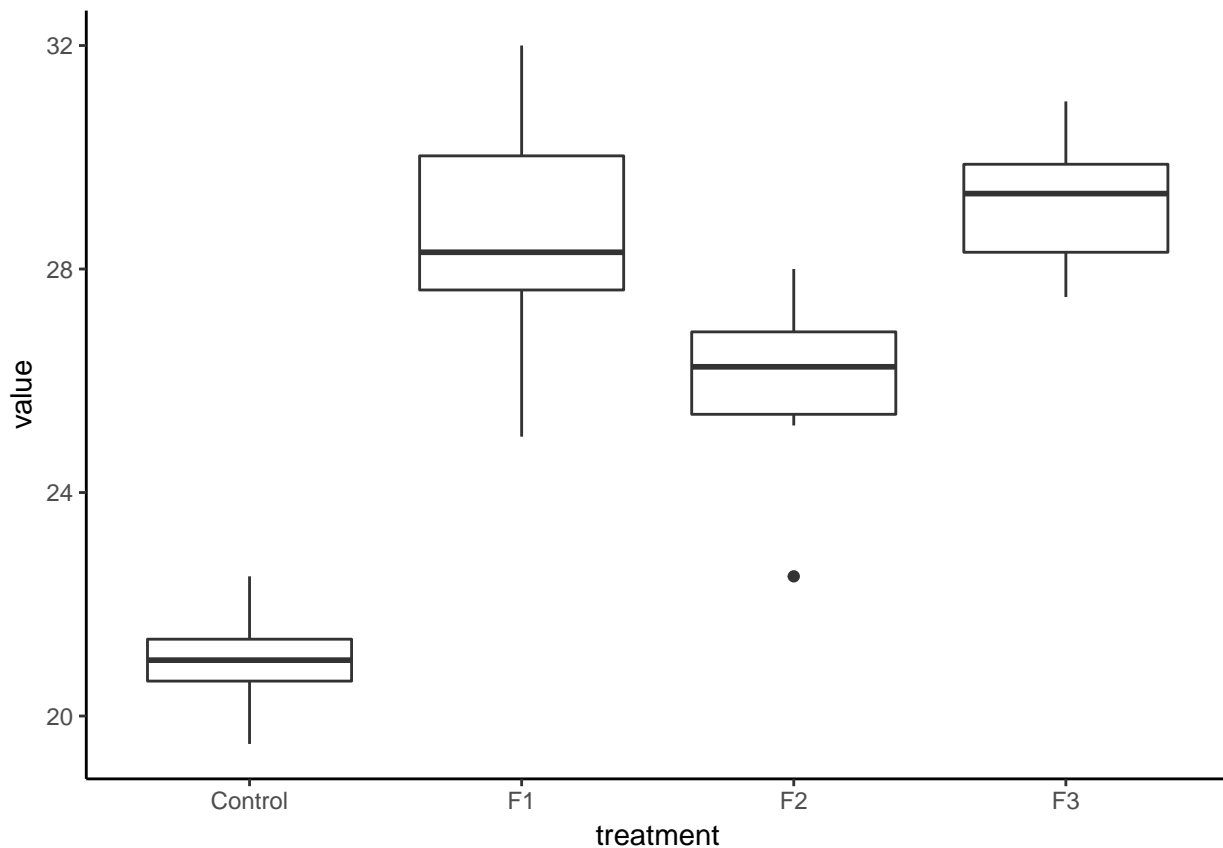
## [1] 26.16667

lesson1_SST <- lesson1_gather %>%
  sum((value - mean(value))^2)

lesson1_SST

## [1] 312.4733

ggplot(lesson1_gather) +
  geom_boxplot(aes(treatment, value)) +
  theme_classic()
```



One-way ANOVA table: Lesson1 Example

Source of Variation	Sum of Squares (SS)	Degrees of Freedom (df)	Mean Squares (MS)	F-Ratio
Between samples	SSB	k - 1	MSB	MSB/MSW
Within samples	SSW	n(total) - k	MSW	
<i>Total</i>	SST = 312.43	n(total) - 1 = 23		

$$\text{Total Sum of Squares } SST = \sum_{i=1}^k \sum_{j=1}^{n_i} (x_{ij} - \bar{\bar{x}})^2$$

$$\text{Sum of Squares Between } SSB = \sum_{i=1}^k n_i (\bar{x}_i - \bar{\bar{x}})^2$$

$$\text{Sum of Squares Within } SSW = SST - SSB \text{ or } SSW = \sum_{i=1}^k \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)^2$$

```
summary_within_groups <- lesson1_gather %>%
  group_by(treatment) %>%
  summarise(N = n(), mean = mean(value)) # SS = (sum( (value - mean(value))^2
```

```
summary_within_groups
```

```
## # A tibble: 4 x 3
##   treatment      N mean
##   <chr>      <int> <dbl>
## 1 Control         6  21.0
## 2 F1              6  28.6
## 3 F2              6  25.9
## 4 F3              6  29.2
```

```
lesson1_SSB <- summary_within_groups %$%
  sum((mean - lesson1_grand_mean)^2)*6
message(cat("SSB ", lesson1_SSB))
```

```
## SSB  251.44
```

```
##
```

```
lesson1_SSW = lesson1_SST - lesson1_SSB
message(cat("SSW ", lesson1_SSW))
```

```
## SSW  61.03333
```

```
##
```

One-way ANOVA table: Lesson1 Example

Source of Variation	Sum of Squares (SS)	Degrees of Freedom (df)	Mean Squares (MS)	F-Ratio
Between samples	SSB = 251.44	k - 1 = 3	83.81	MSB/MSW
Within samples	SSW = 61.03	n(total) - k = 20	3.05	
Total	SST = 312.43	n(total) - 1 = 23		

$$\frac{MSB}{BSW} = \frac{83.81}{3.05} = 27.47$$

Calculate the critical F-statistic (or look it up in a table)

```
qf(0.95, df1=3, df2=20)
```

```
## [1] 3.098391
```

With  $27.47 > 3.1$  we can reject the null hypothesis.

## 7.6 Let's let R do the work:

```
lesson1_aov <- aov(value ~ treatment, lesson1_gather)
summary(lesson1_aov)

##              Df Sum Sq Mean Sq F value    Pr(>F)
## treatment     3  251.44   83.81    27.46 2.71e-07 ***
## Residuals    20   61.03    3.05
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

## 7.7 Which populations have different means?

### 7.7.1 Tukey (or Tukey-Kramer) test

For the example above, we would have constructed the following hypothesis:

$$H_0 : \mu_{control} = \mu_{F1} = \mu_{F2} = \mu_{F3}$$

$$H_a : \text{At least two population means are different.}$$

The ANOVA analysis above only tells us that there is a difference between two or more of the population means.

We could do a pairwise comparison using confidence intervals for each mean; however, this method does not use the entire population variance.

The *Tukey-Kramer procedure for multiple comparisons* is one method to compare two or more groups

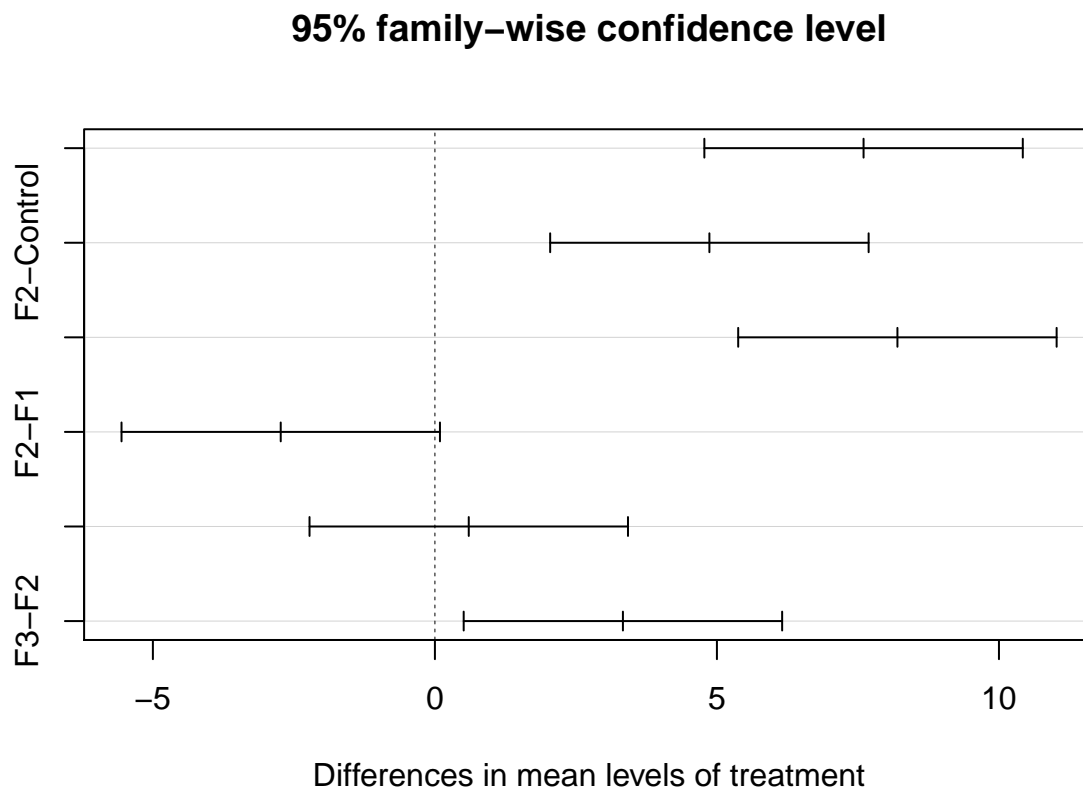
```
lesson1_Tukey <- TukeyHSD(lesson1_aov)
lesson1_Tukey

##      Tukey multiple comparisons of means
##      95% family-wise confidence level
##
## Fit: aov(formula = value ~ treatment, data = lesson1_gather)
##
## $treatment
##              diff              lwr              upr              p adj
## F1-Control    7.600000    4.7770648    10.42293521    0.0000016
## F2-Control    4.866667    2.0437315    7.68960188    0.0005509
## F3-Control    8.200000    5.3770648    11.02293521    0.0000005
## F2-F1         -2.733333   -5.5562685    0.08960188    0.0598655
## F3-F1          0.600000   -2.2229352    3.42293521    0.9324380
## F3-F2          3.333333    0.5103981    6.15626854    0.0171033

library(broom)
tidy(lesson1_Tukey)
```

```
##      term comparison estimate  conf.low  conf.high adj.p.value
## 1 treatment F1-Control  7.600000  4.7770648 10.42293521 1.637988e-06
## 2 treatment F2-Control  4.866667  2.0437315  7.68960188 5.509424e-04
## 3 treatment F3-Control  8.200000  5.3770648 11.02293521 5.148374e-07
## 4 treatment      F2-F1 -2.733333 -5.5562685  0.08960188 5.986551e-02
## 5 treatment      F3-F1  0.600000 -2.2229352  3.42293521 9.324380e-01
## 6 treatment      F3-F2  3.333333  0.5103981  6.15626854 1.710330e-02
```

```
plot(lesson1_Tukey)
```



F3-F2 : a and b

F3-F1 : a

F2-F1 : b

F3-control : c

F2-control : c

F1-control : c

```
summary_lesson1 <- lesson1_gather %>%
  group_by(treatment) %>%
  summarise(N = n(), mean = mean(value), sd = sd(value),
            se = sd/sqrt(N), ci = se*qt(0.975,N-1)) %>%
  mutate(labels = c("c", "ab", "b", "a"))
```

```
summary_lesson1
```

```
## # A tibble: 4 x 7
##   treatment      N  mean    sd   se   ci labels
##   <chr>      <int> <dbl> <dbl> <dbl> <dbl> <chr>
## 1 Control        6  21.0  1.00 0.408  1.05 c
## 2 F1             6  28.6  2.44 0.995  2.56 ab
```

```
## 3 F2          6  25.9  1.90 0.775  1.99 b
## 4 F3          6  29.2  1.29 0.526  1.35 a
```

Shouldn't R be able to do this work for us?

```
library(multcomp)
library(multcompView)

greenhouse_letters <- multcompLetters4(lesson1_aov, lesson1_Tukey)
greenhouse_letters
```

```
## $treatment
##      F3      F1      F2 Control
##      "a"    "ab"    "b"      "c"
```

```
str(greenhouse_letters)
```

```
## List of 1
## $ treatment:List of 3
## ..$ Letters      : Named chr [1:4] "a" "ab" "b" "c"
## .. ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## ..$ monospacedLetters: Named chr [1:4] "a " "ab " " b " " c"
## .. ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## ..$ LetterMatrix    : logi [1:4, 1:3] TRUE TRUE FALSE FALSE FALSE TRUE ...
## .. ..- attr(*, "dimnames")=List of 2
## .. .. ..$ : chr [1:4] "F3" "F1" "F2" "Control"
## .. .. ..$ : chr [1:3] "a" "b" "c"
## ..- attr(*, "class")= chr "multcompLetters"
```

```
library(purrr)
gh_letters_flatten <- greenhouse_letters %>%
  flatten()
str(gh_letters_flatten)
```

```
## List of 3
## $ Letters      : Named chr [1:4] "a" "ab" "b" "c"
## ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## $ monospacedLetters: Named chr [1:4] "a " "ab " " b " " c"
## ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## $ LetterMatrix    : logi [1:4, 1:3] TRUE TRUE FALSE FALSE FALSE TRUE ...
## ..- attr(*, "dimnames")=List of 2
## .. ..$ : chr [1:4] "F3" "F1" "F2" "Control"
## .. ..$ : chr [1:3] "a" "b" "c"
```

```
View(as_tibble(gh_letters_flatten$Letters))
```

```
gh_letters_pluck <- greenhouse_letters %>%
  pluck(1)
str(gh_letters_pluck)
```

```
## List of 3
## $ Letters      : Named chr [1:4] "a" "ab" "b" "c"
## ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## $ monospacedLetters: Named chr [1:4] "a " "ab " " b " " c"
## ..- attr(*, "names")= chr [1:4] "F3" "F1" "F2" "Control"
## $ LetterMatrix    : logi [1:4, 1:3] TRUE TRUE FALSE FALSE FALSE TRUE ...
## ..- attr(*, "dimnames")=List of 2
```

```
## .. ..$ : chr [1:4] "F3" "F1" "F2" "Control"
## .. ..$ : chr [1:3] "a" "b" "c"
## - attr(*, "class")= chr "multcompLetters"
```

```
gh_letters_unlist <- greenhouse_letters %>%
  unlist %>%
  as_tibble()
gh_letters_unlist
```

```
## # A tibble: 20 x 1
##   value
## * <chr>
## 1 a
## 2 ab
## 3 b
## 4 c
## 5 "a "
## 6 "ab "
## 7 " b "
## 8 " c"
## 9 TRUE
## 10 TRUE
## 11 FALSE
## 12 FALSE
## 13 FALSE
## 14 TRUE
## 15 TRUE
## 16 FALSE
## 17 FALSE
## 18 FALSE
## 19 FALSE
## 20 TRUE
```

```
str(gh_letters_unlist)
```

```
## Classes 'tbl_df', 'tbl' and 'data.frame': 20 obs. of 1 variable:
## $ value: chr "a" "ab" "b" "c" ...
```

```
gh_letters_row <- as_tibble(gh_letters_flatten$Letters)
gh_letters_row
```

```
## # A tibble: 4 x 1
##   value
## * <chr>
## 1 a
## 2 ab
## 3 b
## 4 c
```

```
letters_final <- as_tibble(names(greenhouse_letters$treatment[["Letters"]]))
letters_final %<>% rename(treatment = value)
letters_final
```

```
## # A tibble: 4 x 1
##   treatment
##   <chr>
## 1 F3
```

```
## 2 F1
## 3 F2
## 4 Control

final_final <- bind_cols(letters_final, gh_letters_row)
final_final

## # A tibble: 4 x 2
##   treatment value
##   <chr>      <chr>
## 1 F3        a
## 2 F1        ab
## 3 F2        b
## 4 Control   c

# greenhouse1_lm <- lm(value ~ treatment, data = lesson1_gather)
# greenhouse1_lsm <- lsmeans(greenhouse1_lm, ~ treatment)
# greenhouse1_cld <- cld(greenhouse1_lsm, by = NULL, Letters = letters, alpha = .05, reversed = TRUE, me
# greenhouse1_cld
```

## 7.8 ANOVA Block analysis

```
ecoli <- read_table2("Month WR01 WR02 WR03 WR04
March 3. 57.6 12 21.3
April 121. 14.6 6.3 39.9
May 307.6 290.9 290.9 435.2
June 44.1 30.1 34.1 81.3
July 108.1 88 14.8 178.2
August 106.70 146.70 98.70 275.50
September 148.30 517.20 185.00 387.30
October 43.2 81.6 53 198.9", col_names = TRUE)
```

```
ecoli
```

```
## # A tibble: 8 x 5
##   Month      WR01 WR02 WR03 WR04
##   <chr>    <dbl> <dbl> <dbl> <dbl>
## 1 March      3.00 57.6 12.0 21.3
## 2 April     121.  14.6  6.30 39.9
## 3 May       308.  291. 291. 435.
## 4 June      44.1  30.1 34.1 81.3
## 5 July      108.  88.0 14.8 178.
## 6 August    107.  147. 98.7 276.
## 7 September 148.  517. 185. 387.
## 8 October   43.2  81.6 53.0 199.
```

### 7.8.1 Tidy up the data

```
ecoli_tidy <- ecoli %>%
  gather(key = "site", value = "counts", WR01, WR02, WR03, WR04)

ecoli_tidy
```



```
## # A tibble: 32 x 3
##   Month      site counts
##   <chr>    <chr>  <dbl>
## 1 March    WR01     3.00
## 2 April    WR01    121.
## 3 May      WR01    308.
## 4 June     WR01    44.1
## 5 July     WR01    108.
## 6 August   WR01    107.
## 7 September WR01    148.
## 8 October  WR01    43.2
## 9 March    WR02    57.6
## 10 April   WR02    14.6
## # ... with 22 more rows
```

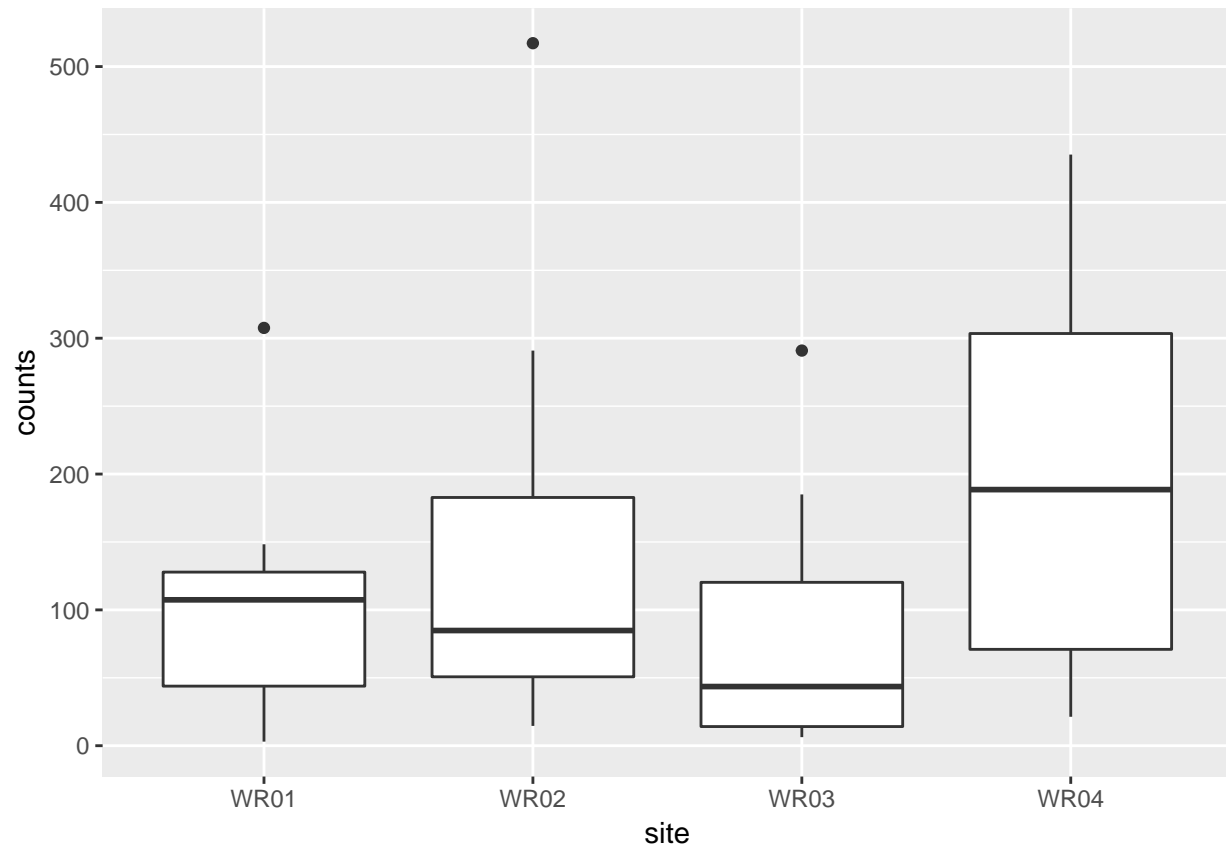
### 7.8.2 One-way ANOVA

```
ecoli_aov <- aov(counts ~ site, data = ecoli_tidy)
summary(ecoli_aov)
```

```
##           Df Sum Sq Mean Sq F value Pr(>F)
## site        3  61945   20648    1.142  0.349
## Residuals   28 506096   18075
```

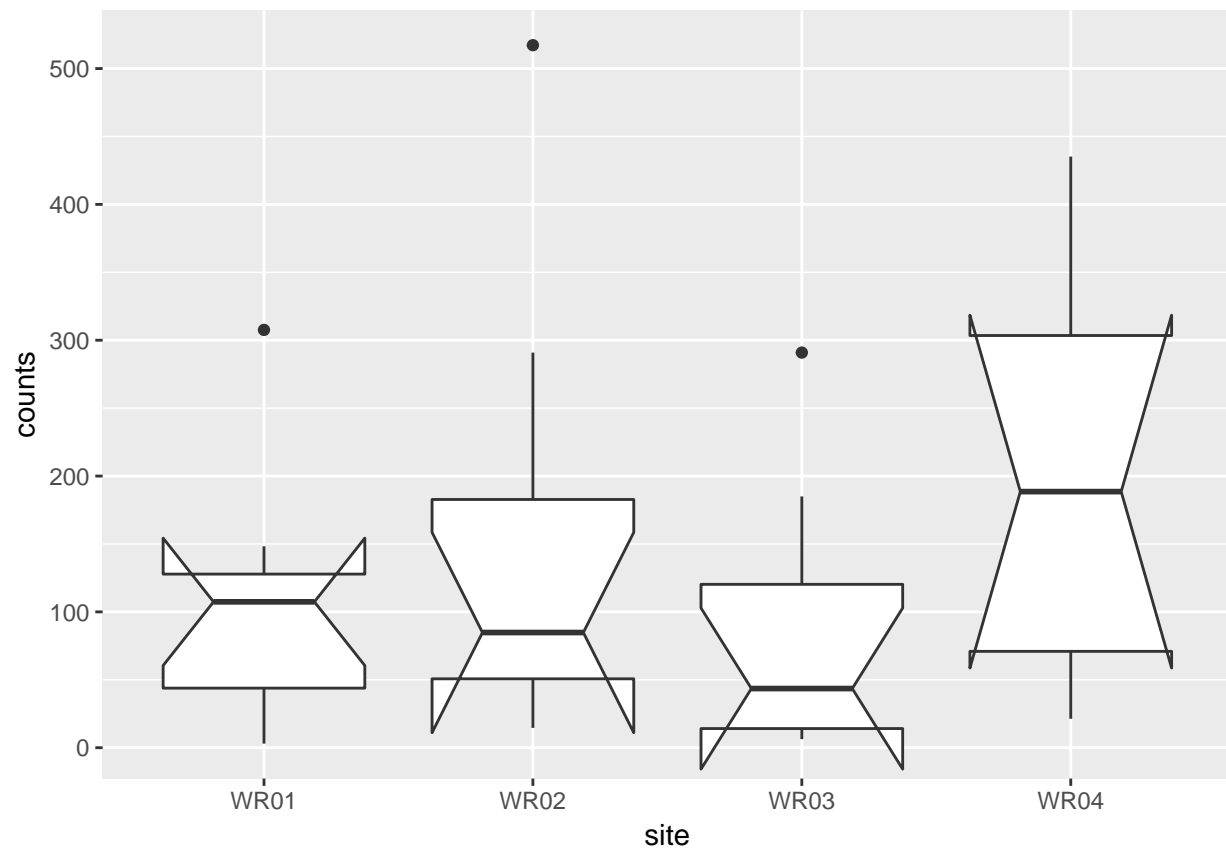
### 7.8.3 Plot of the data

```
ggplot(ecoli_tidy) +
  geom_boxplot(aes(site, counts))
```

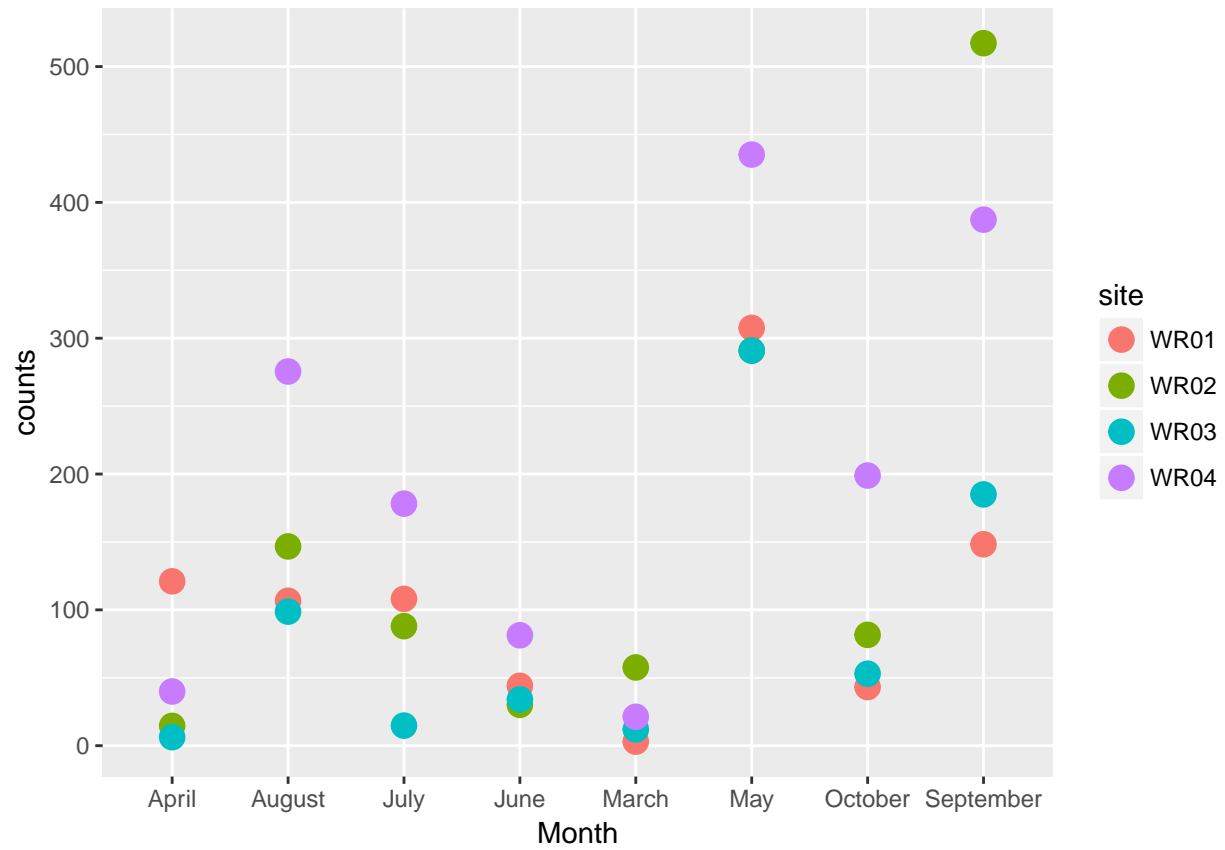


```
ggplot(ecoli_tidy) +  
  geom_boxplot(aes(site, counts), notch = TRUE)
```

```
## notch went outside hinges. Try setting notch=FALSE.  
## notch went outside hinges. Try setting notch=FALSE.  
## notch went outside hinges. Try setting notch=FALSE.  
## notch went outside hinges. Try setting notch=FALSE.
```

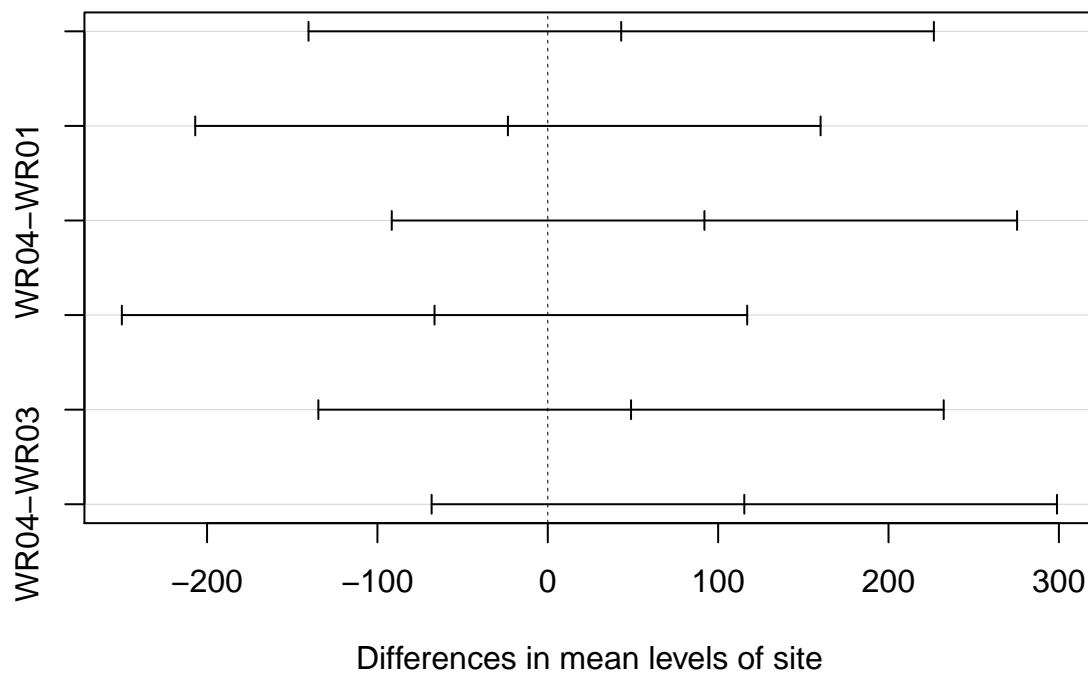


```
ggplot(ecoli_tidy) +  
  geom_point(aes(Month, counts, colour = site), size = 4)
```



```
plot(TukeyHSD(ecoli_aov, conf.level = 0.95))
```

### 95% family-wise confidence level



### 7.8.4 ANOVA with blocking factor

```
ecoli_aov_block <- aov(counts ~ Month + site, data = ecoli_tidy)

summary(ecoli_aov_block)

##           Df Sum Sq Mean Sq F value    Pr(>F)
## Month      7 402112   57445    11.60 5.7e-06 ***
## site       3  61945   20648     4.17 0.0183 *
## Residuals 21 103984    4952
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

### 7.8.5 But what is different?

```
ecoli_block_tukey <- TukeyHSD(ecoli_aov_block, conf.level = 0.95)
ecoli_block_tukey

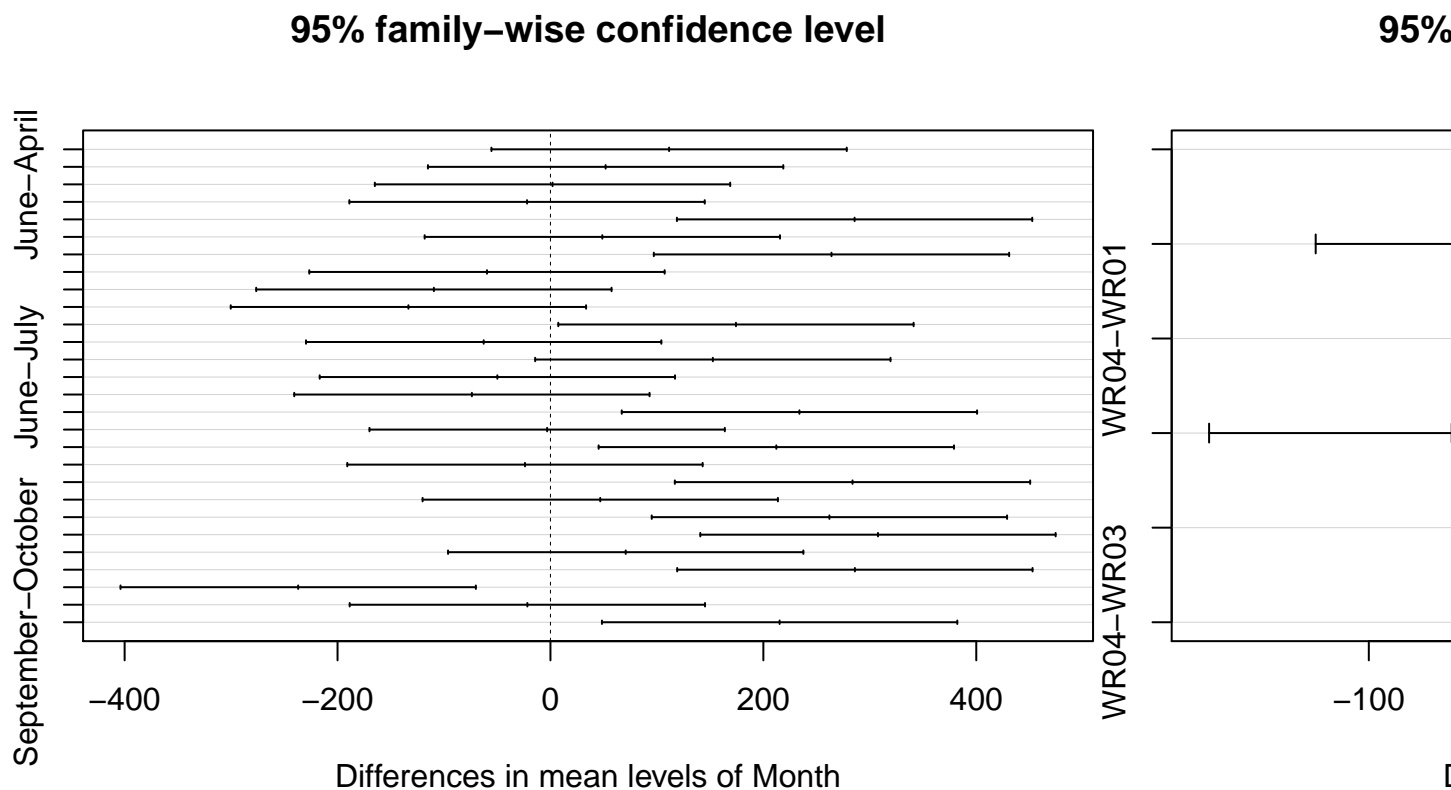
##      Tukey multiple comparisons of means
##      95% family-wise confidence level
##
## Fit: aov(formula = counts ~ Month + site, data = ecoli_tidy)
##
## $Month
##           diff           lwr          upr          p adj
## August-April    111.450   -55.443795  278.34379 0.3691183
## July-April       51.825  -115.068795  218.71879 0.9620137
## June-April        1.950  -164.943795  168.84379 1.0000000
## March-April      -21.975  -188.868795  144.91879 0.9997950
## May-April        285.700   118.806205  452.59379 0.0002417
## October-April    48.725  -118.168795  215.61879 0.9726099
## September-April  264.000    97.106205  430.89379 0.0006458
## July-August      -59.625  -226.518795  107.26879 0.9235806
## June-August     -109.500  -276.393795   57.39379 0.3899013
## March-August    -133.425  -300.318795   33.46879 0.1827645
## May-August       174.250    7.356205  341.14379 0.0366874
## October-August  -62.725  -229.618795  104.16879 0.9032585
## September-August 152.550   -14.343795  319.44379 0.0894265
## June-July        -49.875  -216.768795  117.01879 0.9689635
## March-July       -73.800  -240.693795   93.09379 0.8076556
## May-July         233.875    66.981205  400.76879 0.0025586
## October-July     -3.100  -169.993795  163.79379 1.0000000
## September-July   212.175    45.281205  379.06879 0.0068760
## March-June       -23.925  -190.818795  142.96879 0.9996407
## May-June         283.750   116.856205  450.64379 0.0002639
## October-June     46.775  -120.118795  213.66879 0.9780722
## September-June   262.050    95.156205  428.94379 0.0007058
## May-March        307.675   140.781205  474.56879 0.0000907
## October-March     70.700   -96.193795  237.59379 0.8378113
## September-March  285.975   119.081205  452.86879 0.0002388
## October-May     -236.975  -403.868795  -70.08121 0.0022204
## September-May    -21.700  -188.593795  145.19379 0.9998114
```

```
## September-October 215.275 48.381205 382.16879 0.0059746
##
## $site
##      diff      lwr      upr      p adj
## WR02-WR01 43.0875 -54.981447 141.15645 0.6186609
## WR03-WR01 -23.4000 -121.468947 74.66895 0.9090016
## WR04-WR01 91.9500 -6.118947 190.01895 0.0712136
## WR03-WR02 -66.4875 -164.556447 31.58145 0.2623702
## WR04-WR02 48.8625 -49.206447 146.93145 0.5197897
## WR04-WR03 115.3500 17.281053 213.41895 0.0174029
```

```
multcompLetters4(ecoli_aov_block, ecoli_block_tukey)
```

```
## $Month
##      May September      August      July      October      June      April
##      "a"      "ab"      "bc"      "c"      "c"      "c"      "c"
##      March
##      "c"
##
## $site
## WR04 WR02 WR01 WR03
##      "a" "ab" "ab" "b"
```

```
plot(TukeyHSD(ecoli_aov_block, conf.level = 0.95))
```



## 7.9 Two-way ANOVA with interaction

```
lab_data_2way_anova <- read_table2("46.5    138.4    180.9    39.8    132.4    176.8
                                   47.3 144.4    180.5    40.3    132.4    173.6
                                   46.9 142.7    183 41.2    130.3    174.9", col_names = FALSE)

lab_data_2way_anova
```

```
## # A tibble: 3 x 6
##       X1     X2     X3     X4     X5     X6
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1  46.5  138.  181.  39.8  132.  177.
## 2  47.3  144.  180.  40.3  132.  174.
## 3  46.9  143.  183.  41.2  130.  175.
```

*# I want to stack X1-X3 on top of X4-X6*

```
library(dplyr)
```

```
lab_data_method1 <- lab_data_2way_anova %>%
  dplyr::select(X1:X3) %>%
  rename(dose1 = X1, dose2 = X2, dose3 = X3) %>%
  mutate(method = "method1")
```

```
lab_data_method1
```

```
## # A tibble: 3 x 4
##   dose1 dose2 dose3 method
##   <dbl> <dbl> <dbl> <chr>
## 1  46.5  138.  181. method1
## 2  47.3  144.  180. method1
## 3  46.9  143.  183. method1
```

```
lab_data_method2 <- lab_data_2way_anova %>%
  dplyr::select(X4:X6) %>%
  rename(dose1 = X4, dose2 = X5, dose3 = X6) %>%
  mutate(method = "method2")
```

```
lab_data_method2
```

```
## # A tibble: 3 x 4
##   dose1 dose2 dose3 method
##   <dbl> <dbl> <dbl> <chr>
## 1  39.8  132.  177. method2
## 2  40.3  132.  174. method2
## 3  41.2  130.  175. method2
```

```
lab_data_stack <- bind_rows(lab_data_method1, lab_data_method2)
lab_data_stack
```

```
## # A tibble: 6 x 4
##   dose1 dose2 dose3 method
##   <dbl> <dbl> <dbl> <chr>
## 1  46.5  138.  181. method1
## 2  47.3  144.  180. method1
## 3  46.9  143.  183. method1
## 4  39.8  132.  177. method2
## 5  40.3  132.  174. method2
```

```
## 6 41.2 130. 175. method2
```

```
lab_data_tidy <- lab_data_stack %>%
  gather(key = doping_level, value = conc, dose1, dose2, dose3)
```

```
lab_data_tidy
```

```
## # A tibble: 18 x 3
##   method doping_level conc
##   <chr>    <chr>    <dbl>
## 1 method1 dose1      46.5
## 2 method1 dose1      47.3
## 3 method1 dose1      46.9
## 4 method2 dose1      39.8
## 5 method2 dose1      40.3
## 6 method2 dose1      41.2
## 7 method1 dose2     138.
## 8 method1 dose2     144.
## 9 method1 dose2     143.
## 10 method2 dose2     132.
## 11 method2 dose2     132.
## 12 method2 dose2     130.
## 13 method1 dose3     181.
## 14 method1 dose3     180.
## 15 method1 dose3     183.
## 16 method2 dose3     177.
## 17 method2 dose3     174.
## 18 method2 dose3     175.
```

```
View(lab_data_tidy)
```

```
# run the anova
```

```
lab_data_aov <- aov(conc ~ method + doping_level, lab_data_tidy)
summary(lab_data_aov)
```

```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## method          1     264      264   80.27 3.58e-07 ***
## doping_level    2   57026   28513 8677.63 < 2e-16 ***
## Residuals      14       46        3
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
lab_data_aov_cross <- aov(conc ~ method*doping_level, lab_data_tidy)
```

```
summary(lab_data_aov_cross)
```

```
##              Df Sum Sq Mean Sq  F value    Pr(>F)
## method          1     264      264   98.347 3.92e-07 ***
## doping_level     2   57026   28513 10632.526 < 2e-16 ***
## method:doping_level 2      14        7    2.577  0.117
## Residuals       12      32        3
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```



## Chapter 8

# Assessing Product Reliability

This chapter was not covered in the course and may be added at a later date.



# Bibliography

- Xie, Y. (2015). *Dynamic Documents with R and knitr*. Chapman and Hall/CRC, Boca Raton, Florida, 2nd edition. ISBN 978-1498716963.
- Xie, Y. (2018). *bookdown: Authoring Books and Technical Documents with R Markdown*. R package version 0.7.