IntroSlides with focus on statistics

Basic steps in workflow

- 1. Define environment
- 2. Import
- 3. Transform
- 4. Explore (general/outlier/distribution) (go back to 3?)
- 5. Classify scale level / distribution (based on 3/4)
- 6. Describe
- 7. Test / Model (may include step 6)
- 8. Report

Define environment

- Activate packages to use: library() / pacman::p_load()
- ggplot theme: theme_set() / theme_update()
- flextable settings: set_flextable_defaults()
- knitr::opts_chunk\$set()

```
1 set_flextable_defaults(
2    theme_fun = theme_zebra, font.size = 18, font.family = 'Roboto',
3    table.layout = 'autofit',
4    padding.bottom = .2, padding.top = .2, padding.left = 2, padding.right = 2)
5
6    knitr::opts_chunk$set(message = FALSE, warning = FALSE, comment = NA, echo = T
```

Import

- read_xlsx() / read_csv() / read_csv2()
- options related to separators, number formats, ranges etc.
- rename() / rename_with()

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Glimpse at data: Find the problems?

```
1 head(rawdata, n = 15) |> flextable()|>
                theme zebra(even body = 'aquamarine', odd body = 'antiquewhite')
                                                          WEIGTH OF
                                                                       weight of
                                       ALMINIUM CAP +
                                       WEIGTH OF
                                                                                   weight of
                        WEIGHT OF
                                                                                             MOISTURE
                                                                         sample
CODE CODE OF
                                                                         before sample drying (Wts+d)
                                                                                    sample
                            EMPTY CUP + SAMPLE
                                                      SAMPLE AFTER
                                                                                              CONTENT
OF CUP SAMPLE
                    ALUMINUM(wt)
                                                      DRYING (Wt-AL
                                          (Wt + s)
                                                               +s+d)
                                                                         5.1891
                                                                                     4.6865
69
        D
                            4.1974
                                           9.3865
                                                              4.7000
                                                                                               90.31431
                                                                         5.0770
                            4.1964
                                           9.2734
                                                              4.4670
                                                                                     4.8064
                                                                                               94.67008
        D
                            4.2108
                                           9.2653
                                                                         5.0545
                                                              4.6670
                                                                                     4.5983
                                                                                               90.97438
                                                                                               91.74508
91.58722
                                                              4.6345
114
        D
                            4.2134
                                           9.3146
                                                                         5.1012
                                                                                     4.6801
                                           9.3147
        D
                                                              4.6171
                                                                         5.1291
                                                                                     4.6976
M1
                            4.1856
                                                                                     4.7543
a/17
        D
                            4.2090
                                           9.3204
                                                              4.5661
                                                                         5.1114
                                                                                               93.01366
        D
                            4.1894
                                           9.2661
                                                              4.5778
                                                                         5.0767
                                                                                     4.6883
                                                                                               92.34936
                                                                         5.0912
                                                                                               91.96849
33
                            4.1968
                                           9.2880
        D
                                                              4.6057
                                                                                     4.6823
М
        D
                            4.1535
                                           9.2872
                                                              4.6350
                                                                         5.1337
                                                                                     4.6522
                                                                                               90.62080
E/18/1
                                           9.2476
                                                                                               90.25069
        D
                            4.2534
                                                              4.7403
                                                                         4.9942
                                                                                     4.5073
24/A2
        D
                            4.2066
                                           8.3463
                                                              4.5849
                                                                         4.1397
                                                                                     3.7614
                                                                                               90.86166
13
                            4.1554
                                           9.2384
                                                              4.7402
                                                                         5.0830
                                                                                     4.4982
                                                                                               88.49498
                                           9.2495
                                                                                               89.15458
Хp
        Α
                            4.1893
                                                              4.7381
                                                                         5.0602
                                                                                     4.5114
                                                                         5.1519
                                                                                     4.5233
2p/029
                            4.0654
                                           9.2173
                                                              4.6940
                                                                                               87.79868
                            4.0641
                                           9.2032
                                                              4.8124
                                                                         5.1391
                                                                                     4.3908
                                                                                               85.43908
```

Rename

```
1 colnames (rawdata)
[1] "CODE OF CUP"
[2] "CODE OF SAMPLE"
[3] "WEIGHT OF EMPTY ALUMINUM (wt)"
[4] "WEIGTH OF ALMINIUM CUP + SAMPLE (Wt + s)"
[5] "WEIGTH OF ALUMINIUM CAP + SAMPLE AFTER DRYING (Wt-AL +s+d)"
[6] "weight of sample before drying (Wts)"
[7] "weight of sample after drying (Wts+d)"
[8] "MOISTURE CONTENT (%)"
          1 rawdata <- rawdata |>
              rename(Region=`CODE OF SAMPLE`) |>
              rename with (.fn = ~str replace all (
                c("GTH"="GHT", 'AL.+UM'= 'Cup',
                  'C[UA]P' = 'Cup','\\(\\w+.*\\)'='',
                  'Cup Cup'='Cup',' '=' ')) |>
                  str to title() |> str trim())
          9 cn()
[1] "Code Of Cup"
                                           "Region"
[3] "Weight Of Empty Cup"
                                           "Weight Of Cup + Sample"
[5] "Weight Of Cup + Sample After Drying" "Weight Of Sample Before Drying"
                                         "Moisture Content (%)"
[7] "Weight Of Sample After Drying"
```

Transform

- Change or create columns with mutate() / mutate(across())
- e.g. for log-transformation, creation of factors, text recoding

Code Of Cup	Region	Weight Of Empty Cup	Cup +	+ Sample After Drying	Sample Before Drying	Sample After Drying	Moisture Content (%)	Content (%)
69	D	4.1974	9.3865	4.7000	5.1891	0.5026	90.31431	9.685687
sample 2	D	4.1964	9.2734	4.4670	5.0770	0.2706	94.67008	5.329919
Α	D	4.2108	9.2653	4.6670	5.0545	0.4562	90.97438	9.025621
114	D	4.2134	9.3146	4.6345	5.1012	0.4211	91.74508	8.254920
M1	D	4.1856	9.3147	4.6171	5.1291	0.4315	91.58722	8.412782

Explore / group variables

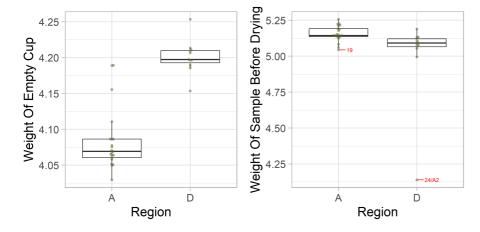
Explore (general/outlier/distribution)

- ggplot()+geom_boxplot() / geom_beeswarm() / geom_density()
- ks.test() / ksnormal() / shapiro.test()

Classify scale level / distribution

- gaussvars / ordvars / factvars, possibly more...
- Store variables accordingly, e.g. ColSeeker()

Explore: Outlier



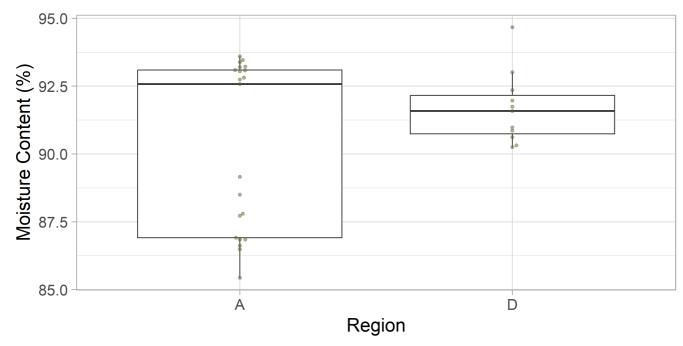
Handle outliers?

Removal is the worst strategy possible, correct errors, think about distributions, winsorize...

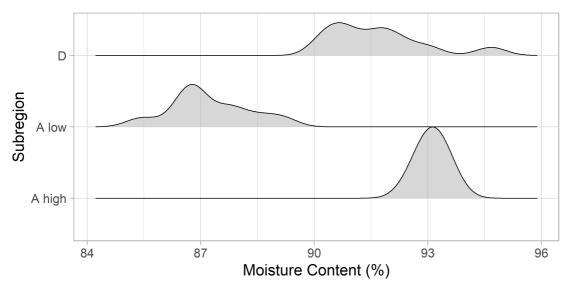


Explore: Unexpecteds

```
1 ggplot(data = rawdata,
2     aes(x = `Region`,
3     y = `Moisture Content (%)`))+
4     geom_boxplot(outlier.alpha = 0) +
5     geom_beeswarm(alpha=.5, color="darkolivegreen")
```



Transform Subregions?



Explore: Normal distribution 1

- Gaussian Normal distribution is required for many statistical procedures
- Common tests are graphical exploration, Shapiro-Wilk-test and Kolmogorov-Smirnov-test

```
1 p_normal <-
2    shapiro.test(x = rawdata$`Moisture Content (%)`)
3 p_normal</pre>
```

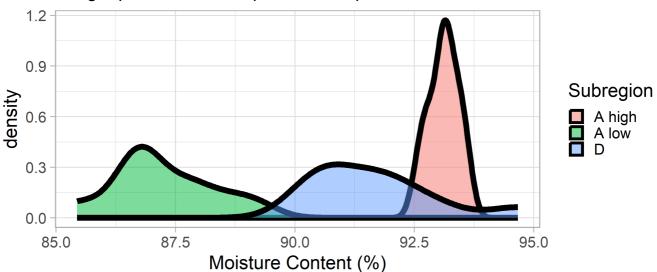
```
Shapiro-Wilk normality test

data: rawdata$`Moisture Content (%)`
W = 0.89133, p-value = 0.003752
```

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p (Shapiro) global = 0.004

A high: p=0.923; A low: p=0.756; D: p=0.207



Explore: Normal distribution 2

```
\# A tibble: 7 \times 4
                                     `A high` `A low`
 Variable
                                     <chr> <chr> <chr>
1 Weight Of Empty Cup
                                    0.989 n.s. 0.444 n.s. 0.697 n.s.
2 Weight Of Cup + Sample
                                    0.785 n.s. 0.980 n.s. 0.019 *
3 Weight Of Cup + Sample After Drying 0.900 n.s. 0.710 n.s. 0.969 n.s.
4 Weight Of Sample Before Drying 0.196 n.s. 0.999 n.s. 0.072 +
5 Weight Of Sample After Drying
                                    0.976 n.s. 0.555 n.s. 1.000 n.s.
6 Moisture Content (%)
                                    0.975 n.s. 0.733 n.s. 0.954 n.s.
7 Dry Content (%)
                                    0.975 n.s. 0.733 n.s. 0.954 n.s.
```

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Explore: Group variables by type/distribution

Scale level determines what statistics are appropriate Typical scale levels are

- nominal/categorical/factorial/qualitative: just different groups (species, eye color, genotype, treatment)
- ordered categories: few groups with inherent order (quality bad<medium<good, pain between 0 and 10)
- ordinal measures: many different values, natural order, no distribution assumption (satisfaction on a scale from 0 to 100)
- measures following a Normal distribution
- possibly measures from other known distributions (beta, log-normal, poisson...), often treated as ordinal

Make type decision obvious/reproducible

```
1 gaussvars <- ColSeeker(data=rawdata,namepattern = c('Weight','Content'))</pre>
            gaussvars
$index
[1] 3 4 5 6 7 8 9
$names
[1] "Weight Of Empty Cup"
                                           "Weight Of Cup + Sample"
[3] "Weight Of Cup + Sample After Drying" "Weight Of Sample Before Drying"
                                       "Moisture Content (%)"
[5] "Weight Of Sample After Drying"
[7] "Dry Content (%)"
$bticked
[1] "`Weight Of Empty Cup`"
[2] "`Weight Of Cup + Sample`"
[3] "`Weight Of Cup + Sample After Drying`"
[4] "`Weight Of Sample Before Drying`'
[5] "`Weight Of Sample After Drying`"
         1 ordvars <- ColSeeker(namepattern='Weight.+Sample', exclude = 'After')</pre>
          2 ordvars$names
[1] "Weight Of Cup + Sample"
                                      "Weight Of Sample Before Drying"
          1 factvars <- ColSeeker(namepattern='region', casesensitive = FALSE)</pre>
          2 factvars$bticked
[1] "`Region`"
                 "`Subregion`"
```

Model

Describe

- mean() / sd() / meansd()
- median() / quantile() / median_quart()
- table() / prop.table() / cat_desc_stats()

Test

- t.test() / lm()+[Aa]nova() / compare2numvars()
- wilcox.test()
- fisher.test() / glm(family=binomial)

Model: Describe

Sample size n: per variable, if there are NAs

Mean: central tendency, the expected typical

value

$$\frac{\sum x}{n}$$

Variance: measure for

variability/heterogeneity of data

$$\frac{\sum (x - mean)^2}{n - 1}$$

Standard deviation SD: the *typical* weighted

deviation from the mean

$$\sqrt{Var}$$

Standard error of the mean SEM: how reliable is the mean *estimate*, what would be the expected SD of means from repeated experiments?

$$\frac{SD}{\sqrt{n}}$$

Median: Split between lower/upper 50% of data

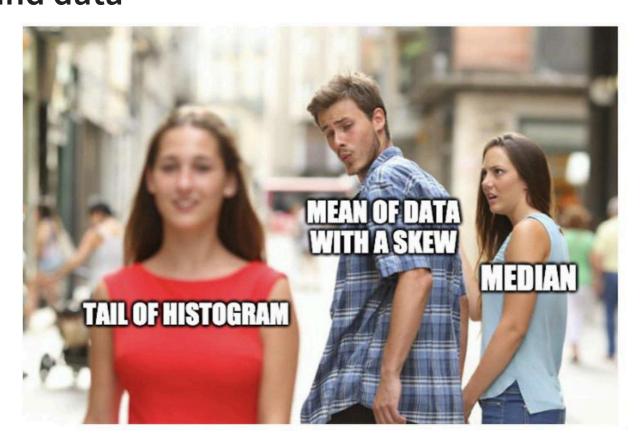
Quartiles: Split at 25%/50%/75% of data (more

general: Quantiles, e.g.Percentiles), used in boxplot

various computational approaches

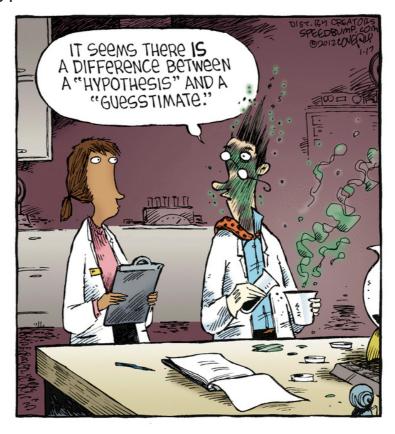
```
1 desc_gauss <- rawdata |>
         2 summarize(across(.cols = gaussvars$names,
                             .fns = meansd))
         4 desc gauss
# A tibble: 1 × 7
  `Weight Of Empty Cup` `Weight Of Cup + Sample` Weight Of Cup + Sample After \dots^1
              <chr>
                                                <chr>
                       9.2 \pm 0.2
1 \ 4.1 \pm 0.1
                                                4.6 \pm 0.1
# i abbreviated name: 1`Weight Of Cup + Sample After Drying`
\sharp i 4 more variables: `Weight Of Sample Before Drying` <chr>,
    `Weight Of Sample After Drying` <chr>, `Moisture Content (%)` <chr>,
   `Dry Content (%) ` <chr>
          1 desc ord <- rawdata |>
          2 summarize(across(ordvars$names,.fns=~median_quart(.x,roundDig = 3))) |>
             pivot longer(everything(),
                          names to = 'Measure', values to = 'Median[1Q/3Q]')
         5 desc ord
\# A tibble: 2 × 2
                                `Median[1Q/3Q]`
 Measure
                                <chr>
  <chr>
1 Weight Of Cup + Sample 9.25 (9.22/9.29)
2 Weight Of Sample Before Drying 5.14 (5.09/5.18)
```

Descriptive Stats should match distribution and data



Model: Test

Tests require hypotheses



Null hypothesis?

- Working hypothesis: This is what you expect!
 E.g. treatment is lowering blood pressure more than placebo,
 transgenic animals become obese, bio reactor A is more efficient than
 B, concentration of substance is correlated with speed of reaction ...
- Null hypothesis: This is what you test!
 No difference / relation, BP under therapy = BP under placebo

4 possibilities:

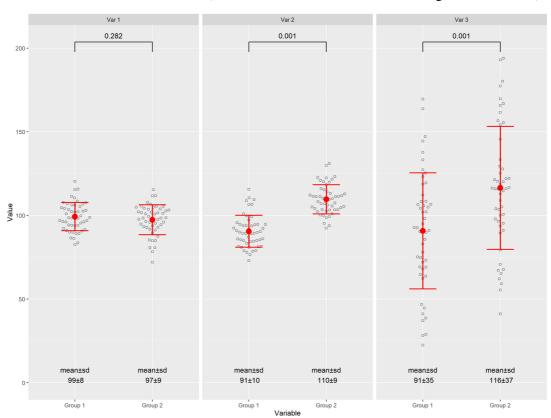
- Null hypothesis correct, test false positive (case A): alpha-error
- Null hypothesis correct, test correct negative (case B)
- Null hypothesis false, test false negative (case C): beta-error
- Null hypothesis false, test correct positive (case D)

Significance: NOT probability of case A, but probability of your data given the NULL hypothesis, calculated from your data, conventionally <0.05

Power: Probability of case D, *estimated* based on assumptions about effects and sample size, *calculation* would require knowledge of true difference, conventionally set at 0.80

Test functions

t-test / Wilcoxon-test (aka Mann-Whitney U-test)



t-test

- Assumptions: Continuous data with Normal distribution
- 1 or 2 (independent or dependent) samples with/without equal variances
- how big is the mean difference relative to uncertainty?
 t = (mean₁ mean₂)/SEM
- t follows a t-distribution, allows estimation of probability of t under the NULL hypothesis

Wilcoxon-test

- nonparametric, no distribution is assumed
- based on rank-transformed data
- insensitive to extreme values

Test examples: single variables

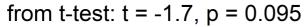
```
Welch Two Sample t-test
```

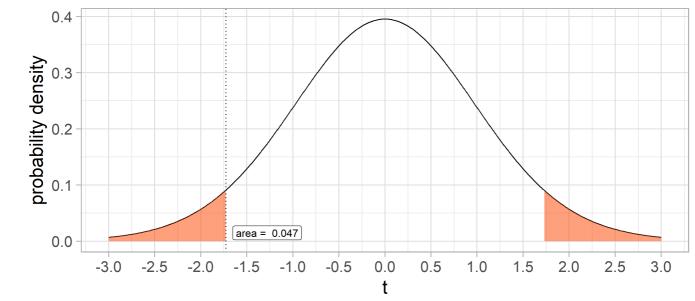
```
1 #Wilcoxon-Test
2 wilcox.test(`Moisture Content (%)`~`Region`,
3 data = rawdata)
```

Wilcoxon rank sum exact test

```
data: Moisture Content (%) by Region W=107, p-value = 0.7547 alternative hypothesis: true location shift is not equal to 0
```

From t to p





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Model: Test 2 / multiple variables

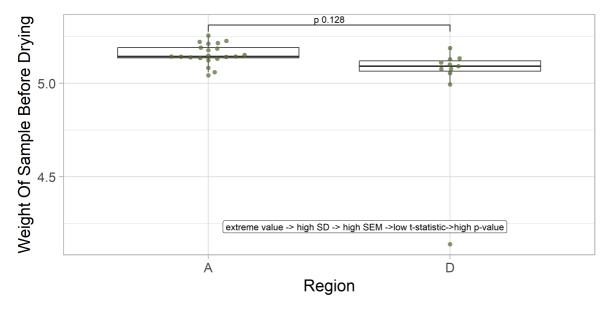
```
Variable
                                                 desc_all
                                                                Region A
                                                                               Region D
Weight Of Empty Cup
                                                 4.1 ± 0.1
                                                                4.1 \pm 0.0
                                                                               4.2 \pm 0.0
                                                                                              0.00001
Weight Of Cup + Sample 9.2 \pm 0.2
Weight Of Cup + Sample After Drying 4.6 \pm 0.1
Weight Of Sample Before Drying 5.1 \pm 0.2
Weight Of Sample After Drying 0.47 \pm 0.
                                                                               9.2 \pm 0.3
                                                                9.2 ± 0.0
                                                                                              0.74227
                                                                                              0.42213
                                                                4.6 \pm 0.2
                                                                               4.6 ± 0.1
                                                Moisture Content (%)
                                                9.2 ± 2.7
                                                               9.7 ± 3.1
                                                                               8.3 \pm 1.3
Dry Content (%)
```

 Variable
 desc_all
 Region A
 Region D
 p

 Weight Of Cup + Sample
 9.25 (9.22/9.29) 9.24 (9.22/9.25) 9.29 (9.27/9.31) 0.003

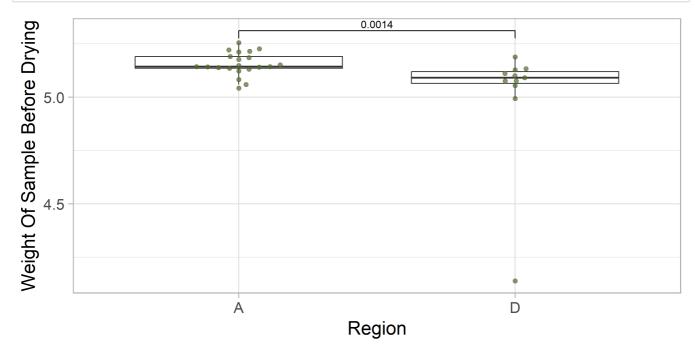
 Weight Of Sample Before Drying
 5.14 (5.09/5.18) 5.14 (5.13/5.20) 5.09 (5.06/5.13) 0.001

Show results



Re-thinking test decision?

```
1 ggplot(rawdata, aes(x = `Region`,y = `Weight Of Sample Before Drying`))+
2    geom_boxplot(outlier.alpha = 0)+
3    geom_beeswarm(alpha=.7, size=2,cex = 2, color="darkolivegreen")+
4    geom_signif(comparisons = list(c(1,2)),test = wilcox.test)
```

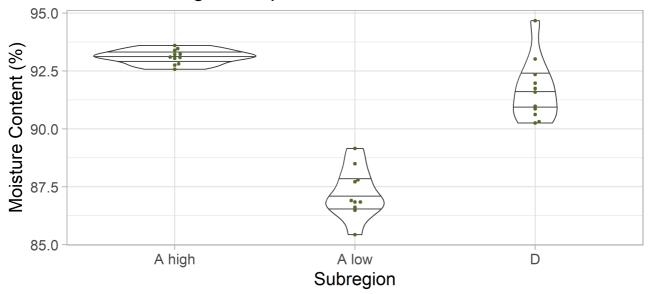


Model: linear models 1 / univariable

```
plottmp <- ggplot(rawdata,aes(Subregion,`Moisture Content (%)`))+
geom_violin(draw_quantiles = c(.25,.5,.75))+
geom_beeswarm(color="darkolivegreen")+

ggtitle('Are all Subregions equal?')
print(plottmp)</pre>
```

Are all Subregions equal?



ANOVA: build model

```
1 rawdata |> group_by(Subregion) |>
2  summarize(MeanMoisture=mean(`Moisture Content (%)`) |> roundR(4)) |>
3  pivot_wider(names_from = Subregion, values_from = MeanMoisture) |>
4  rename_with(~paste('Mean moisture %\n',.x)) |> flextable()|>
5  theme_zebra(even_body = 'aquamarine',odd_body = 'antiquewhite')
```

Mean moisture % Mean moisture % Mean moisture % A high A low D 93.11 87.23 91.67

```
1 lm1<- lm(`Moisture Content (%)`~Subregion, data=rawdata)
2 lm1</pre>
```

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ANOVA: get p-values

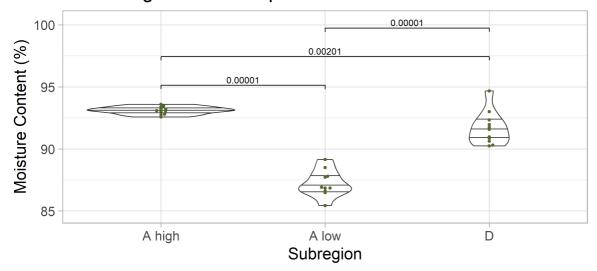
```
1 anova(lm1) |> broom::tidy() |> flextable()|>
2 theme_zebra(even_body = 'aquamarine',odd_body = 'antiquewhite')
```

term df sumsq meansq statistic p.value Subregion 2 194.34239 97.1711969 97.76477 0.00000000000001292127 Residuals 29 28.82393 0.9939285

```
A low "0.00001" " NA"
D "0.00201" "0.00001"
```

Visualize ANOVA

All Subregions are unequal

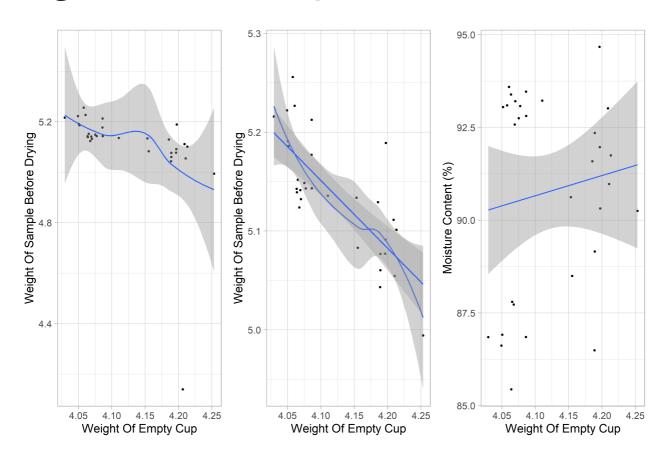


Analyze more than 1 outcome

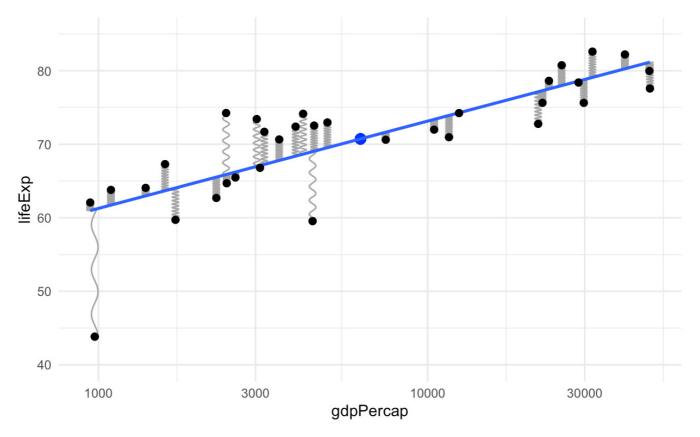
Variable	Subregion A high	Subregion A low	Subregion D	multivar_p
Weight Of Empty Cup	4.1 ± 0.0 c	4.1 ± 0.1 c	4.2 ± 0.0	0.001
Weight Of Cup + Sample	9.2 ± 0.0	9.2 ± 0.0	9.2 ± 0.3	0.894
Weight Of Cup + Sample After Drying	4.4 ± 0.0 bc	$4.8 \pm 0.1 c$	4.6 ± 0.1	0.001
Weight Of Sample Before Drying	5.2 ± 0.0	5.1 ± 0.1	5.0 ± 0.3	0.095
Weight Of Sample After Drying	0.36 ± 0.02 bc	0.66 ± 0.06 c	0.42 ± 0.07	0.001
Moisture Content (%)	93 ± 0 bc	87 ± 1 c	92 ± 1	0.001
Dry Content (%)	7 ± 0 bc	13 ± 1 c	8 ± 1	0.001

b indicates difference from group 2, c indicates difference from group 3

Regression: Scatterplot



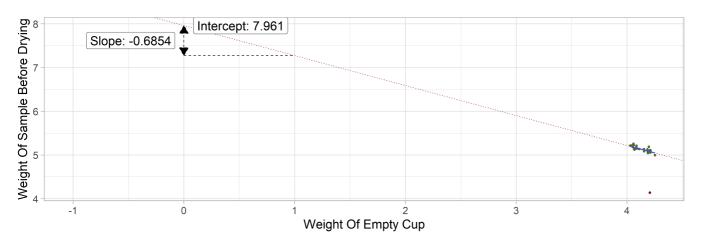
Regression: Underlying mechanics



Regression: Statistics

```
1 lm out0 <- lm(`Weight Of Sample Before Drying` ~ `Weight Of Empty Cup`,
                         data=rawdata)
          3 lm_out0
lm(formula = `Weight Of Sample Before Drying` ~ `Weight Of Empty Cup`,
   data = rawdata)
Coefficients:
          (Intercept) `Weight Of Empty Cup`
               10.169
                                      -1.228
          1 # filtering outlier
          2 lm_out <- lm(`Weight Of Sample Before Drying` ~ `Weight Of Empty Cup`,</pre>
                         data=rawdata |> filter(`Weight Of Sample Before Drying`>4.5))
          4 lm_out
lm(formula = `Weight Of Sample Before Drying` ~ `Weight Of Empty Cup`,
   data = filter(rawdata, `Weight Of Sample Before Drying` >
       4.5))
Coefficients:
          (Intercept) `Weight Of Empty Cup`
               7.9612
                                     -0.6854
```

Regression: Visualize



Regression: Significance

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Report

- RMarkdown and quarto are powerful tools to create reports and presentations
- Export figures: ggsave() / png() / pdf()
- Export tables: write_xlsx()
- Package flextable provides nice features for table formatting

Flextable example

```
1 test_ord |> select(-desc_all) |> rename_with(~str_remove(.,'Code Of ')) |>
2    flextable() |>
3    theme_zebra(even_body = 'aquamarine',odd_body = 'antiquewhite')|>
4    italic(~p<=0.05,j = 1) |> bg(~p<=0.05,j = 4,bg = 'yellow') |>
5    set_caption('Treatment effects, measures following a normal distribution') |
6    add_footer_lines('Significance level is set at 0.05') |>
7    fontsize(size = 12,part = 'footer')
```

 Variable
 Region A
 Region D
 p

 Weight Of Cup + Sample
 9.24 (9.22/9.25) 9.29 (9.27/9.31) 0.003

 Weight Of Sample Before Drying
 5.14 (5.13/5.20) 5.09 (5.06/5.13) 0.001

 Significance level is set at 0.05

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Useful tools along the way

- Pick columns / rows: select() / pull() / filter() / slice()
- Change format of tibble wide <-> long (e.g. for repeated measures): pivot_longer()/pivot_wider()
- Regular expressions: str_replace() / str_detect() / str_...
- Merge text elements: paste() / str_glue()
- Apply functions: purrr::map_xxx