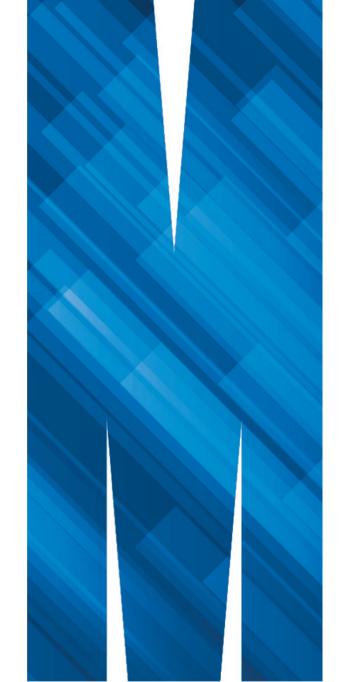


# Visualising experimental designs with the edibble and deggust R-packages

Presenter: Emi Tanaka

- ≤ emi.tanaka@monash.edu
- ¥ @statsgen
- # 11 Nov 2021 @ Applications of Statistical Procedures in Biological Data



# **"I today's menu**



Experimental design in reality •





Grammar of graphics with ggplot2 🔤 🕨



Visualising experimental designs with deggust 😐 🕨

These slides made using R powered by HTML/CSS/JS can be found at emitanaka.org/slides/stats4bio2021/deggust

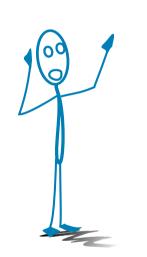


# **Experimental design in reality**

# An experiment generally involves more than one

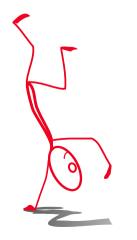
person

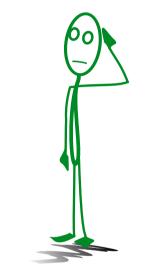
# Meet the cast starring today



The "statistician"

The **"domain expert**"





The "technician"

The "analyst"

Stick person images by OpenClipart-Vectors from Pixabay



The **"domain expert"** drives the experimental objective and has the intricate knowledge about the subject area

The "domain expert"



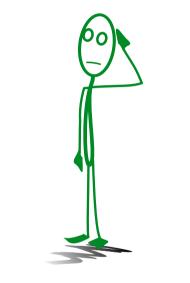
The **"statistican**" creates the experimental design layout after taking into account the statistical and practical constraints.

The **"analyst**" analyses the data after the data is collected.

The "statistician"

The "analyst"

The "**technician**" carries out the experiment and collects the data.

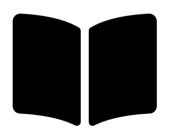


The "technician"

# See the props



The statistical software to design experiments





The software to enter and store data

Good old pen and paper

Missing prop: the statistical software to analyse experimental data

### The actors are purely illustrative.

In practice:

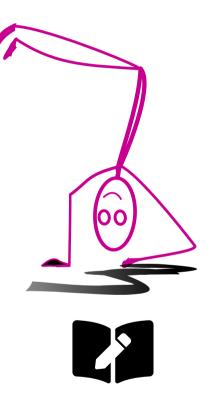
- multiple people can take on each role,
- one person can take on multiple roles, and/or
- a person in the role may not specialise in that role (e.g. the statistician role can be acted out by a non-statistician).



### How we expect experiments are run

Hey, I need to run an experiment. Can you test irrigation and fertilizer effect on plant growth? Bla bla bla...

> Okay. I got the experimental structure perfectly. I'll go generate the experimental design layout.



### How we expect experiments are run

00

I have a *complete* understanding of the experimental structure so I shall enter it in the software to generate the experimental design



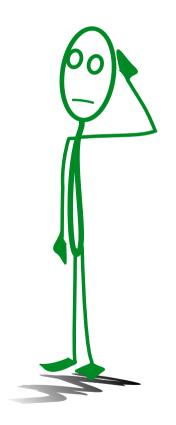
### How we expect experiments are run

Here is the design layout

00

I'll execute this experiment exactly as planned and enter the data with absolutely no mistake





### But

*communication is complex, fraught with tensions, misunderstandings, and problems — rather than a simple process of creating shared meaning — Littlejohn et al. (2017)* 

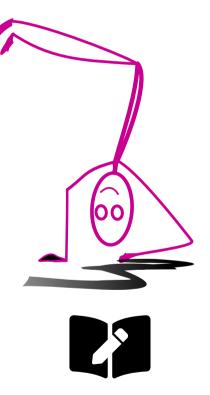
Littlejohn, Stephen W., Karen A. Foss, and John G. Oetzel. 2017. Theories of Human Communication. Waveland Press, Inc.

14/64

• Misunderstandings or incomplete understandings

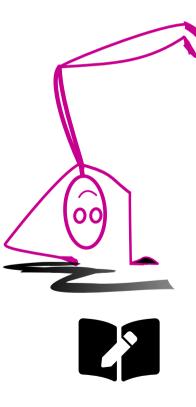
Hey, I need to run an experiment. Can you test irrigation and fertilizer effect on plant growth? Bla bla bla...

Okay. I think I got it. I'll go see what we can do for the experimental design.



• A lot of back-and-forth to be on the same page

(which is completely natural and okay)



Okay how about this plan.



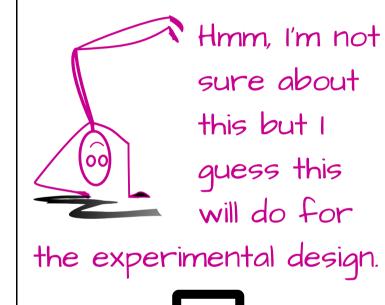
Actually, we can't apply different irrigation methods to these set of plots so we have to change this part. Bla bla.

Okay, I'll write this in my notebook.

OR limited communication and decisions made in silo



well, we'll just leave that empty when we get the plan.



Hmm, I'm not sure about this but I quess this will do for



Oh no! One side of the green house gets more sunlight than the other! Let's move the pots around so that they get the same amount of sunlight.

• Implicit decisions never explicitly transcribed

Why is the experimental design like this?

I think I had a good reason at the time but I can't remember!



Why are we always on a handstand anyway?

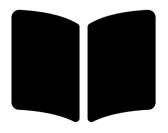
There's no good reason for that!

Knowledge lost



How was the experimental design constructed?

The statistician left a bunch of notes before leaving us for another position but 1 don't know what's what, so 1 don't know.



• Thinking analysis will save you



I think we may have data quality issues in this experimental data. Oh cool data! I can try this fancy statistical model! Hmm, what did you say?

I'm saying that the data may be rubbish. But I got some numbers from fitting this model. 100)

# Garbage in, garbage out

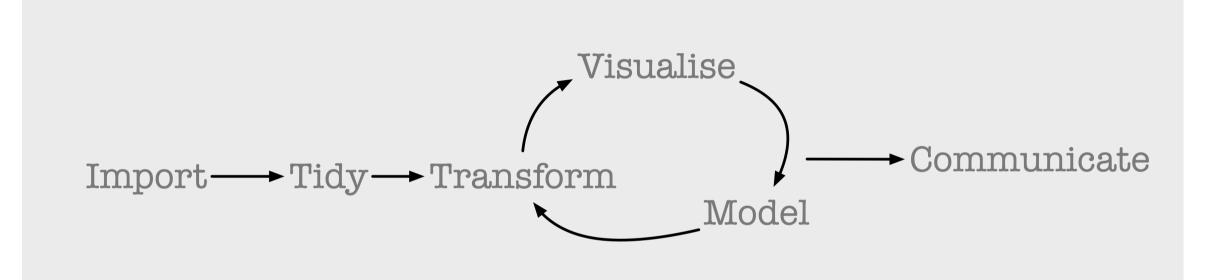
No statistical model, however complex it is, can make any sense of the data if the collected data is rubbish

# Redoing an experiment is expensive

There's a higher stake in getting the experiment design wrong compared to getting the analysis wrong.

In some cases, redoing an experiment is not every possible!

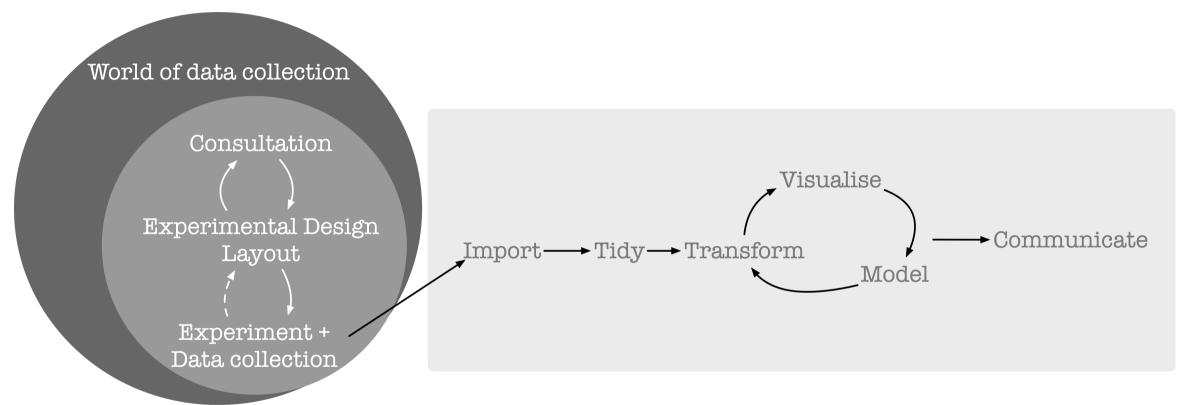
#### What most statistics (and data science) research is about



(with disproportionate amount in Model)

### World of data collection

But there is a whole world of data collection before importing data!



- There is probably more gain in extracting information in ensuring the quality of the data than analysis.
- Experimental design research is generally concerned about generating the experimental design layout
- edibble aims to complement many great experimental design research to design the whole experiment



# Overview of edibble

### The grammar of experimental designs

An abstract computational framework that maps fundamental experimental components to an object oriented system to build and modify experimental designs. Currently implemented as the edibble R-package.



### **R** Package documentation:

edibble.emitanaka.org

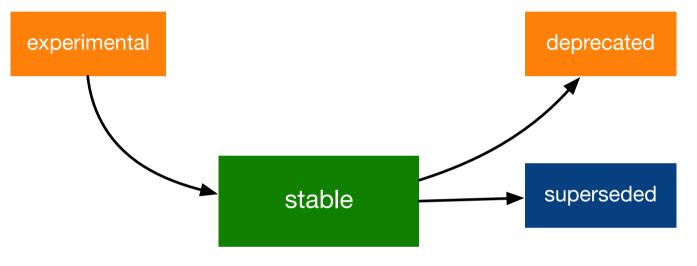
### Source code:

github.com/emitanaka/edibble

Name origin: Opposite produce experimental design table (or tibble)

#### Lifecycle

### https://lifecycle.r-lib.org/articles/stages.html



- Currently edibble is lifecycle experimental
- Some functions like allocation\_trts and randomise\_trts have become lifecycle deprecated in favour of allot\_trts and assign\_trts

Lionel Henry and Hadley Wickham (2021). lifecycle: Manage the Life Cycle of your Package Functions. R package version 1.0.1. https://CRAN.R-project.org/package=lifecycle

### Reframing how you think about experimental designs

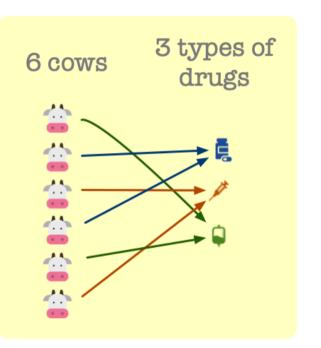
"

Good design considers units and treatments first, and then allocates treatments to units. It does not choose from a menu of named designs.

-Rosemary Bailey (2008)

- edibble encourages users to think about designs exactly as Bailey (2008) suggests
- Nevertheless named experimental designs are very prevelant and can be useful to describe particular designs succintly!
- So let's have the best of both worlds

### Example 1 Completely randomised design



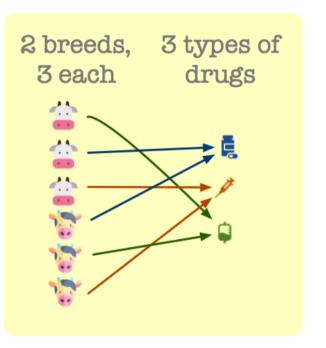
#### library(edibble)

```
code_classical("crd", t = 3, n = 6)
```

```
set.seed(648)
start_design("crd") %>%
set_units(unit = 6) %>%
set_trts(treat = 3) %>%
allot_trts(treat ~ unit) %>%
assign_trts("random") %>%
serve_table()
```

- Note: currently only limited named experimental designs are supported
- A this function name and arguments will likely change in near future

### Example 2 Randomised complete block design



### library(edibble)

```
code_classical("rcbd", t = 3, b = 2)
```

• A this function name and arguments will likely change in near future

### Example 3 Factorial design

#### library(edibble)

code\_classical("factorial", trt = c(2, 4), n = 16)

• **A** this function name and arguments will likely change in near future

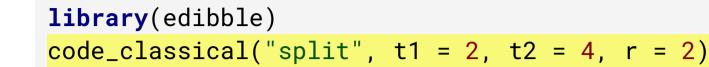
### Example **4** Split-plot design

irrigation system

4 varieties of carrots

🍇 🇞 🍫 💊

rainfed



• **A** this function name and arguments will likely change in near future

### Example **G** Sptrip-plot design



```
library(edibble)
start_design("Strip-plot") %>%
  set_trts(diet = 4,
           breed = 5) %>%
  set_units(hen = 5,
            order = 4,
            chick = ~hen:order) %>%
  allot_trts(breed ~ hen,
             diet ~ order) %>%
  assign_trts("random") %>%
  serve_table()
## # An edibble: 20 x 5
```

##		diet	breed	hen	order	chick
##		<trt(4)></trt(4)>	<trt(5)></trt(5)>	<unit(5)></unit(5)>	<unit(4)>	<unit(20)></unit(20)>
##	1	diet1	breed3	hen1	order1	chick1
##	2	diet1	breed4	hen2	order1	chick2
##	3	diet1	breed1	hen3	order1	<b>chick3</b> 33/64

### **Experimental context is important**

• Name the variables so it always reminds you of the context

## # An edibble: 16 x 4 ## mainplot subplot water variety <unit(4)> <unit(16)> <trt(2)> <trt(4)> ## ## 1 mainplot1 subplot1 irrigated variety3 2 mainplot1 subplot2 irrigated variety1 ## irrigated variety4 3 mainplot1 subplot3 ## ## 4 mainplot1 subplot4 irrigated variety2 ## 5 mainplot2 subplot5 irrigated variety2 ## 6 mainplot2 subplot6 irrigated variety4

```
## # An edibble: 16 x 4
##
                            diet
                                    breed
           pen
                     COW
##
     <unit(4)> <unit(16)> <trt(2)> <trt(4)>
##
   1
                   cow1 low-card
                                   breed3
          pen1
##
   2
                   cow2 low-card
                                   breed1
          pen1
##
   3
                   cow3 low-card
                                   breed4
          pen1
##
   4
          pen1
                   cow4
                        low-card
                                   breed2
##
   5
                   cow5 low-card
                                   breed2
          pen2
                                   breed4 34/64
##
                        low-card
   6
          pen2
                   соwб
```

#### Example 6 Calf feeding experiment

 3 feed types

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

 •••

## Loading required package: openxlsx

## Wagga Wagga

## ✓ Calf feeding has been written to 'calf-design.xlsx'

### Example 7 Chick weight

- An experiment was conducted on a prairie in Western Canada to find out if insecticides used to control grasshoppers affected the weight of young chicks of ring-necked pheasants, either by affecting the grass around the chicks or by affecting the grasshoppers eaten by the chicks.
- Three insecticides were used, at low and high doses.
- The low dose was the highest dose recommended by the department of agriculture; the high dose was four times as much as the recommended dose, to assess the effects of mistakes.
- The experimental procedure took place in each of three consecutive weeks.
- On the first day of each week a number of newly-hatched female pheasant chicks were placed in a brooder pen.
- On the third day, the chicks were randomly divided into twelve groups of six chicks each.
- Each chick was given an identification tape and weighed.
- On the fourth day, a portion of the field was divided into three strips, each of which was divided into two swathes.
- The two swathes within each strip were sprayed with the two doses of the same insecticide.

- Two pens were erected on each swathe, and one group of pheasant chicks was put into each pen.
- For the next 48 hours, the chicks were fed with grasshoppers which had been collected locally.
- Half the grasshoppers were anaesthetized and sprayed with insecticide; the other half were also anaesthetized and handled in every way like the first half except that they were not sprayed.
- All grasshoppers were frozen.
- The experimenters maintained a supply of frozen grasshoppers to each pen, putting them on small platforms so that they would not absorb further insecticide from the grass.
- In each swathe, one pen had unsprayed grasshoppers while the other had grasshoppers sprayed by the insecticide which had been applied to that swathe.
- At the end of the 48 hours, the chicks were weighed again individually.



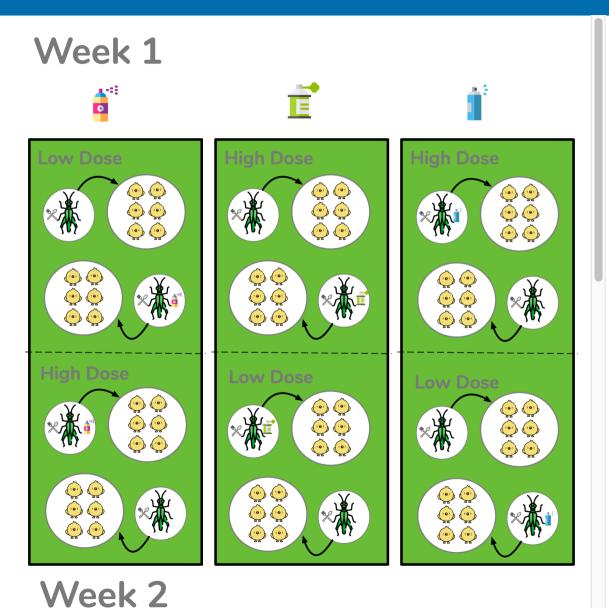
## Example 7 Chick weight: the edibble code

```
start_design("Chick weight") %>%
  set_trts(insecticide = 3,
           dose = c("low", "high")) %>%
  set_units(week = 3,
            strip = nested_in(week, 4),
            swathes = nested_in(strip, 2),
            pen = nested_in(swathes, 2),
            chick = nested_in(pen, 6)) %>%
  set_trts(food = c("spray", "no-spray")) %>%
  allot_trts(insecticide ~ strip,
             dose \sim swathes,
             food ~ pen) %>%
  assign_trts("random") %>%
  set_rcrds(weight = chick) %>%
  serve_table()
## # An edibble: 288 x 9
```

## insecticide dose week strip swathes pen

37/64

# Example 7 Chick weight: closer look



Skel	Skeleton ANOVA					
	Stratum	Source	df			
	Week	Week	2			
	Strips	Insecticide	2			
		Strips Residual	4			
	Swathes	Dose	1			
		Insecticide : Dose	2			
		Swathes Residual	6			
	Pens	Food	1			
		Insecticide : Food	2			
		Dose : Food	1			
		Insecticide : Dose : Food	2			
		Pens Residual	12			
	Chicks (OU)	OU Residual	180			

38/64

All designs thus far have been **balanced** (i.e. equal replicate) and **complete** (each treatment appears the same number of times in each block)...

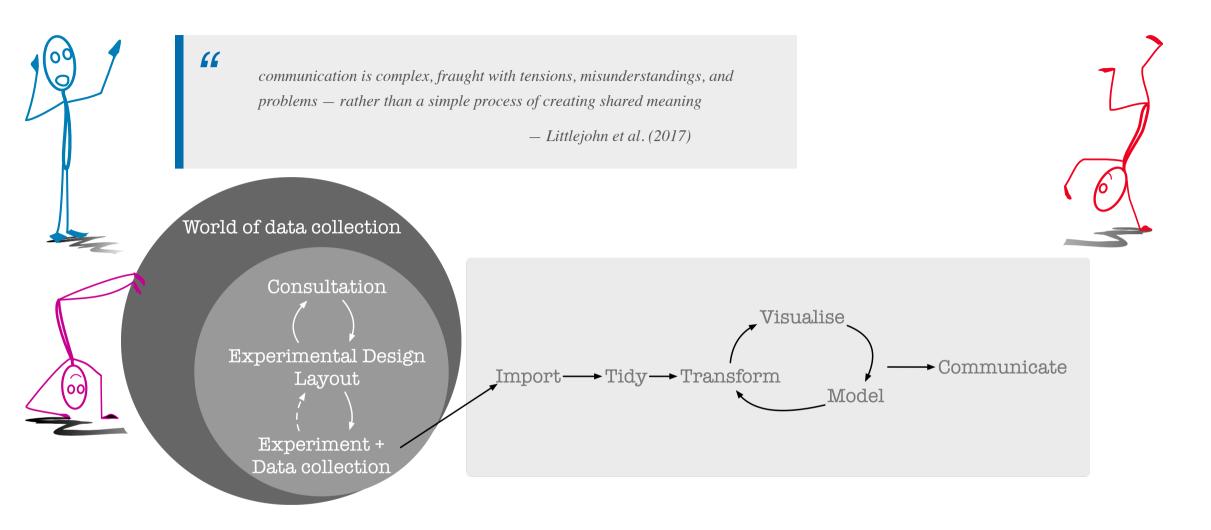
# What about unbalanced and/or incomplete designs?

Reference level by its name:

serve\_table()

Reference level by number:

serve\_table()



# What can help to communicate more effectively?



# Grammar of graphics with ggplot2

# Grammar of graphics: origin and implementations

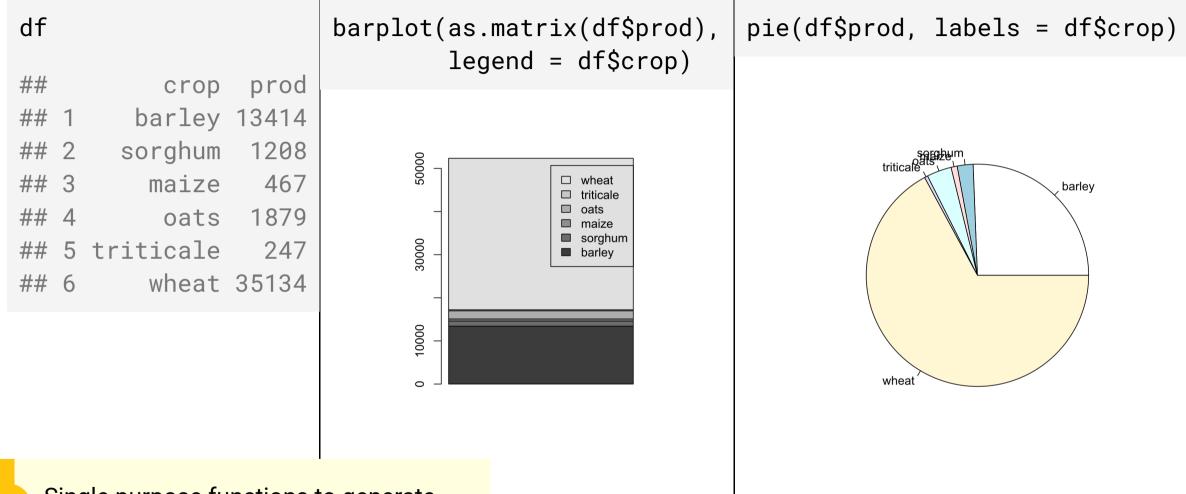
- Initial instances of the grammar of graphics was mentioned by William C. Brinton
- A full computational framework was developed by Leland Wilkinson with implementation in **SYSTAT**.
- An interpretation of the grammar of graphics by Hadley Wickham (as part of his PhD, 2008) was implemented in R as the ggplot2 package.
- Emulation of ggplot2 in **python** started to be developed:
  - ggpy (defunct)
  - plotnine by Hassan Kibirige,
  - seaborn by Michael Waskom (this one is not quite trying to emulate ggplot)
- In **Julia**, **Gadfly** by Daniel C. Jones implements the grammar of graphics.
- In Matlab, gramm by Pierre Morel implements the grammar as a toolbox.
- In Javascript, G2 by AntV team, adding also interactivity, with this version emulated in R as g2r package.
- ggplot2 is arguably the most popular interpretation of grammar of graphics with over 35,000 citations

# **Data 1 Crop production in Australia**

In Australia, total production of each crop nationally are

Crop	Production ('000t)
barley	13,414
sorghum	1,208
maize	467
oats	1,879
triticale	247
wheat	35,134

# **Plotting with "base R"**



Single purpose functions to generate "named plots"

R Core Team (2020) R: A Language and Environment for Statistical Computing https://www.R-project.org/

# Plotting with the ggplot2 R-package

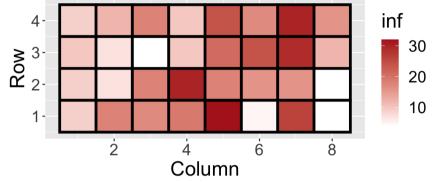
df ## crop prod ## 1 barley 13414	<pre>ggplot(df, aes(x = "", # dummy</pre>	<pre>ggplot(df, aes(x = "", # dummy</pre>				
<pre>## 2 sorghum 1208 ## 3 maize 467 ## 4 oats 1879 ## 5 triticale 247 ## 6 wheat 35134</pre>	5000 40000 30000 20000 10000 0 	<pre>coord_polar(theta = "y") </pre>				
The difference between a <b>stacked barplot</b> and a <b>pie chart</b> is that the coordinate system is transformed from the						

Cartesian coordinate to polar coordinate.

# Making publication ready plots with ggplot2

```
ggplot(cochran.crd, aes(col, row, fill = inf)) +
geom_tile(color = "black", size = 1.3) +
scale_fill_gradient(low = "white", high = "firebrick")
labs(title = "Potato scab infection with sulfur\ntreatm
    x = "Column", y = "Row",
    caption = "Data source: Tamura, R.N. and Nelson, L
theme(text = element_text(size = 20),
    plot.caption = element_text(size = 12),
    plot.title.position = "plot",
    plot.caption.position = "plot",)
```

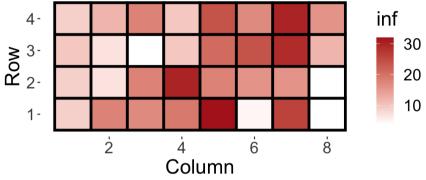
Potato scab infection with sulfur treatments



Data source: Tamura, R.N. and Nelson, L.A. and Naderman, G.C., (1988). An investigation of the validity and usefulness of trend analysis for field plot data. Agronomy Journal, 80, 712-718.

# Making publication ready plots with ggplot2

Potato scab infection with sulfur treatments

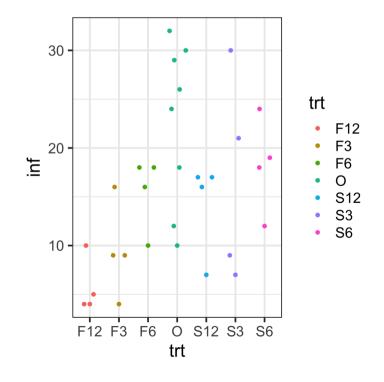


Data source: Tamura, R.N. and Nelson, L.A. and Naderman, G.C., (1988). An investigation of the validity and usefulness of trend analysis for field plot data. Agronomy Journal, 80, 712-718.

## Many extension packages exists for ggplot2

# https://exts.ggplot2.tidyverse.org/gallery/

```
ggplot(cochran.crd, aes(trt, inf, color = trt)) +
    ggbeeswarm::geom_quasirandom() +
    theme_bw(base_size = 18)
```





# Visualising experimental

# designs with the deggust R-

package

# **Visualising experimental designs**

The deggust R-package aims to convert edibble designs to ggplot objects seamlessly.

Currently under developed!

**R** Package documentation:

deggust.emitanaka.org

Source code:

github.com/emitanaka/deggust

Name origin: deggust as in degust, and
make design of experiments into ggplot objects





# **Example: Pig diet experiment**

```
library(edibble)
plan <- start_design("Pig diet experiment") %>%
  set_trts(diet = c("carb", "protein", "fat")) %>%
  set_units(pig = 50) %>%
  allot_trts(diet ~ pig) %>%
  assign_trts("random", seed = 1) %>%
  serve_table()
```

#### plan

##	# /	An edibbl	e: 50 x 2
##		diet	pig
##		<trt(3)></trt(3)>	<unit(50)></unit(50)>
##	1	carb	pig1
##	2	carb	pig2
##	3	protein	pig3
##	4	carb	pig4
##	5	protein	pig5

# Visualising designs with ggplot2

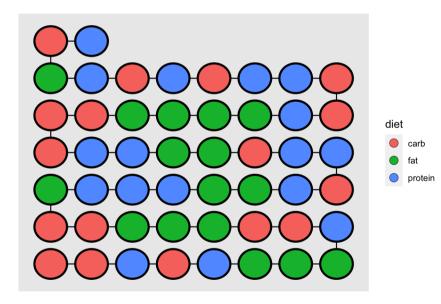
```
library(ggplot2)
plan %>%
  edibble::as_data_frame() %>% # in the future this step will not be needed
ggplot(aes(pig, "1", fill = diet)) +
geom_tile(color = "black")
```

- Slightly painful if you want to quickly visualise your design.
- Also not a great visualisation

Just autoplot it!

library(deggust)

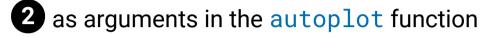
autoplot(plan)



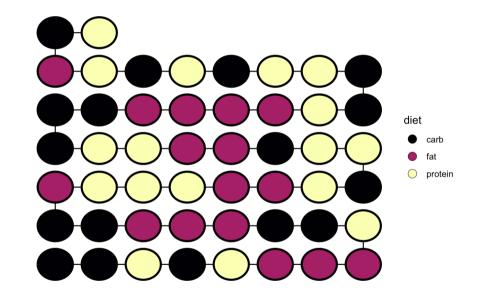
- It makes some decision for you of how to plot which can be customised in two ways:
  - 1 modify scale and theme like any ggplot objects!
  - **2** as arguments in the autoplot function

• It makes some decision for you of how to plot which can be customised in two ways:

modify scale and theme like any ggplot objects!



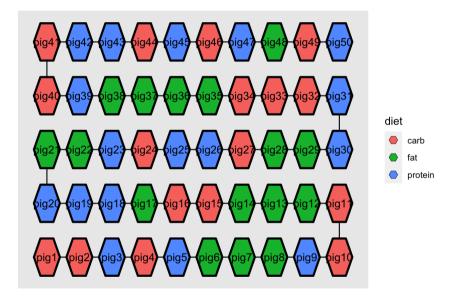
```
autoplot(plan) +
    # ggplot2 functions below
    theme_void() +
    scale_fill_viridis_d(option = "A")
```

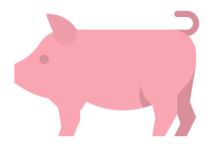


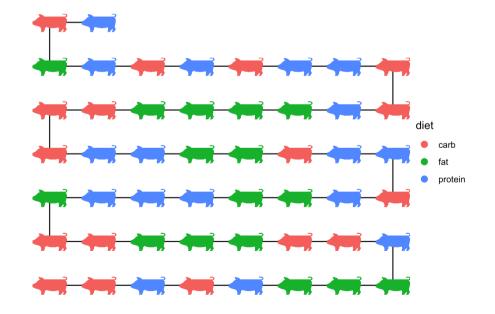
• It makes some decision for you of how to plot which can be customised in two ways:

modify scale and theme like any ggplot objects!

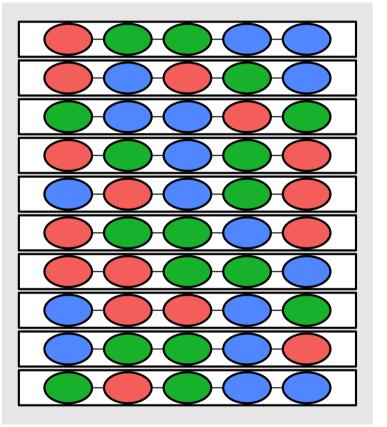
**2** as arguments in the autoplot function





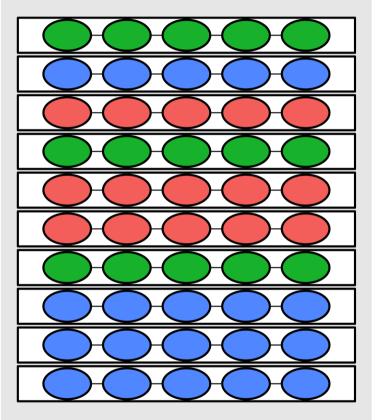


Nested design



breed A B C

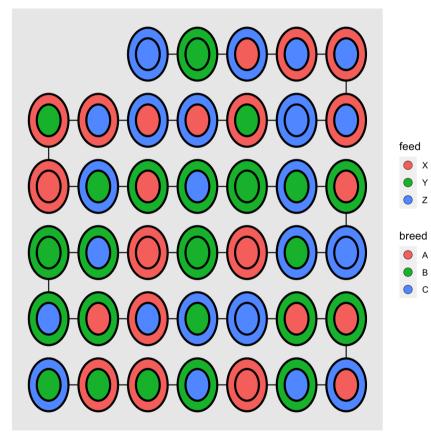
• What changed here?



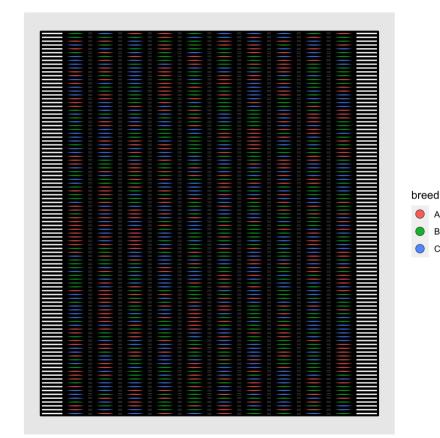
• Factorial experiment

```
start_design() %>%
   set_units(pig = 40) %>%
   set_trts(breed = c("A", "B", "C"),
        feed = c("X", "Y", "Z")) %>%
   allot_trts(breed:feed ~ pig) %>%
   assign_trts("random", seed = 2021) %>%
   serve_table() %>%
   autoplot()
```

• Note: scale will be fixed so it's easier to distinguish between different treatment factors

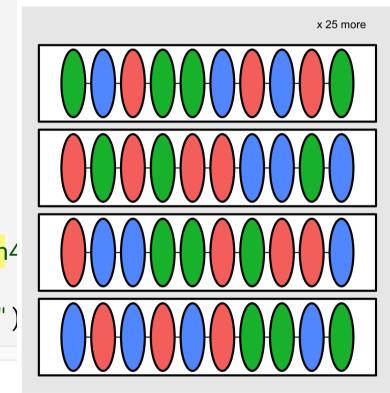


• Is your design too big to fit in the plot?



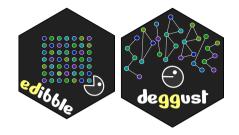
- Is your design too big to fit in the plot?
- Subset it!

```
start_design() %>%
 set_units(pen = 100,
            pig = nested_in(pen, 10)) %>%
 set_trts(breed = c("A", "B", "C")) %>%
 allot_trts(breed ~ pig) %>%
 assign_trts("random", seed = 2021) %>%
 serve_table() %>%
 dplyr::filter(pen %in% c("pen1", "pen2", "pen3", "pen4
 autoplot() +
 annotate("text", x = 10, y = 4.7, label = "x 25 more")
```



### Summary

- The grammar of experimental designs is an abstract computational framework that encourages a higher-order thinking by enforcing the experimental structure and context
- edibble is designed to be user friendly and accommodate natural order of thinking for specifying experimental structure
- The grammar makes each step modular... you can easily extend it (like deggust) or mix-and-match methods
- This makes it easier to leverage existing functionalities in edibble so other developers can focus on what they want to do the most
- And hopefully this framework becomes a common base that promotes collaboration and knowledge sharing



#### World of data collection

Consultation

Experimental Design Layout

> Experiment + Data collection

# Thanks for listening!

- **S** Slides: emitanaka.org/slides/stats4bio2021/deggust
- **R** edibble package documentation: edibble.emitanaka.org
- edibble source code: github.com/emitanaka/edibble
- **R** deggust package documentation: deggust.emitanaka.org
- O deggust source code: github.com/emitanaka/deggust
- emi.tanaka@monash.edu 🕑 @statsgen
- Feature requests or issues with edibble or deggust? Submit or upvote here: github.com/emitanaka/edibble/issues, github.com/emitanaka/deggust/issues, send me an email or tell me now!