

Grammar of Experimental Design

実験計画法の「文法」

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 @statsgen

 23 Jan 2021 @ TokyoR



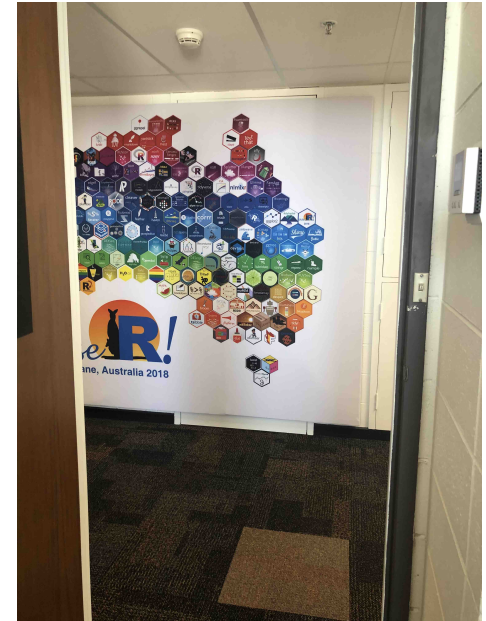
A little about me

自己紹介

- オーストラリア育ちの日本語がイマイチなJapanese-Australianです🇯🇵🇦🇺
- 5年前に統計学の博士号を取得しました🎓
- Monash大学で働くため2020年1月シドニーからメルボルンへ引っ越しました📦



私のオフィスからの見晴らしです➡



その研究内容一つとは

Grammar of Experimental Design

実験計画法の「文法」

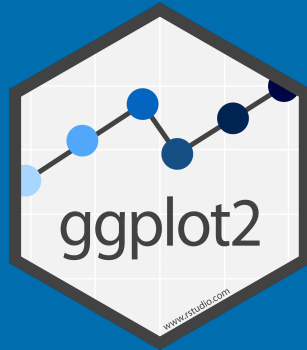
「文法」とはどのような意味なのでしょう？

内容

- ①  **Grammar of Graphics** グラフィックスの文法
- ②  **Grammar of Data Manipulation** データ操作の文法
- ③  **Grammar of Experimental Design** 実験計画法の文法

1

Grammar of Graphics



Wickham (2016) ggplot2: Elegant Graphics for Data Analysis. *Springer-Verlag New York*

Wilkinson (2005) The Grammar of Graphics. *Statistics and Computing. Springer, 2nd edition.*

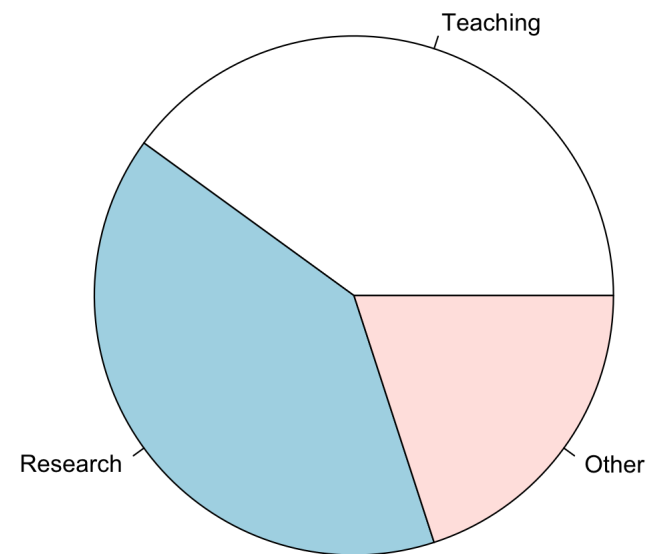
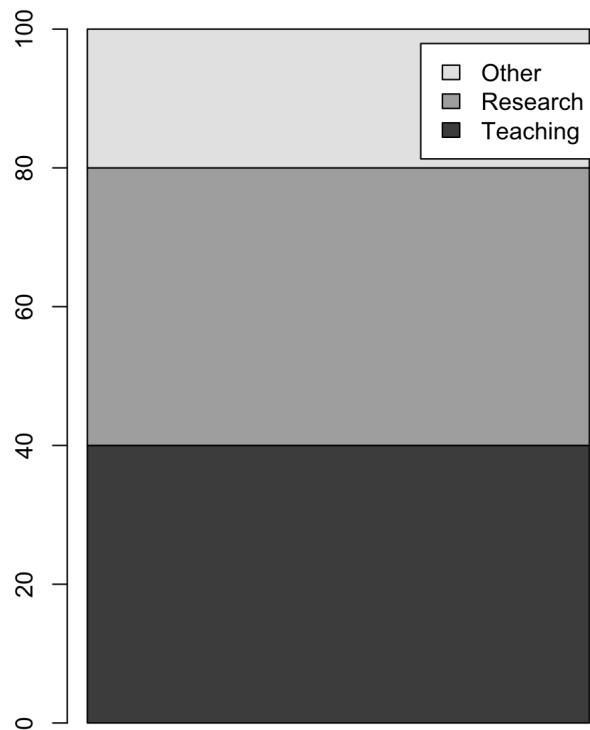
まずはデーターから



一般的なオーストラリアの大学で働いてる学者は時間を以下のように分けるよう期待されています：

- 40%教育、
- 40%研究と
- 20%その他。

この二つのプロットの違いとは？



Base R

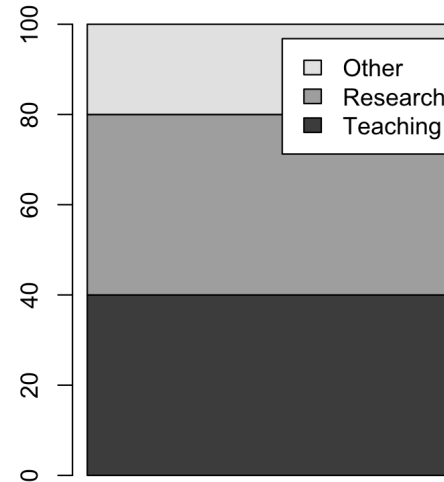
```
df

##      duty perc
## 1 Teaching  40
## 2 Research  40
## 3   Other   20

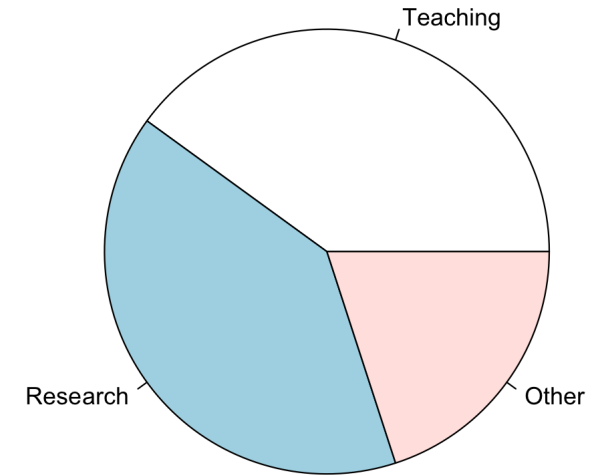
tibble::as_tibble(df)

## # A tibble: 3 x 2
##   duty      perc
##   <chr>    <dbl>
## 1 Teaching    40
## 2 Research    40
## 3   Other     20
```

```
barplot(as.matrix(df$perc),
        legend = df$duty)
```



```
pie(df$perc, labels = df$duty)
```



Single purpose functions
to generate "named plots"

ggplot2

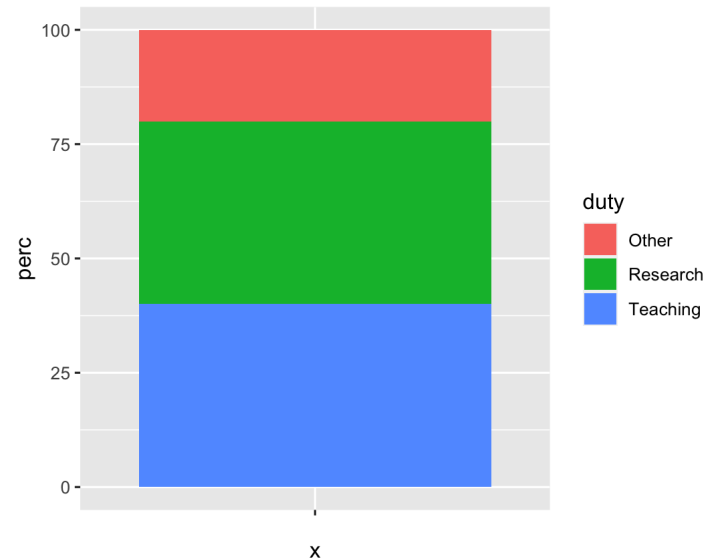
```
df
```

```
##           duty perc
## 1 Teaching    40
## 2 Research    40
## 3   Other     20
```

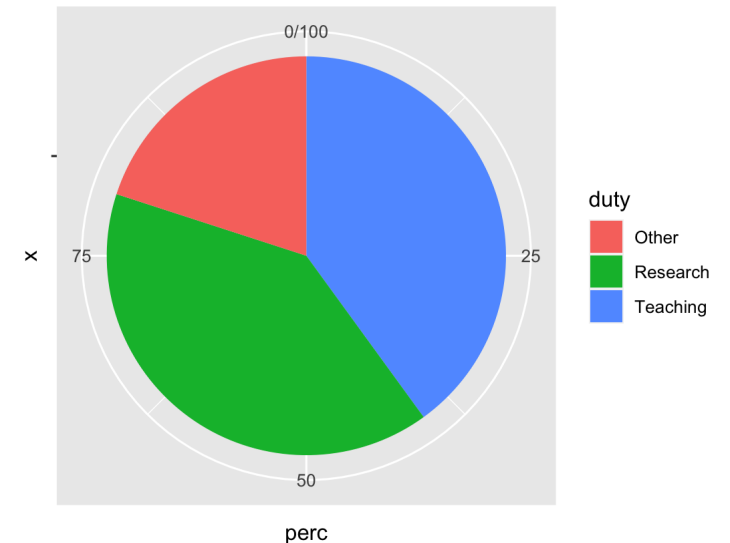
```
tibble::as_tibble(df)
```

```
## # A tibble: 3 x 2
##   duty      perc
##   <chr>    <dbl>
## 1 Teaching    40
## 2 Research    40
```

```
ggplot(df, aes(x = "", # dummy
               y = perc,
               fill = duty)) +
  geom_col()
```



```
ggplot(df, aes(x = "", # dummy
               y = perc,
               fill = duty)) +
  geom_col() +
  coord_polar(theta = "y")
```



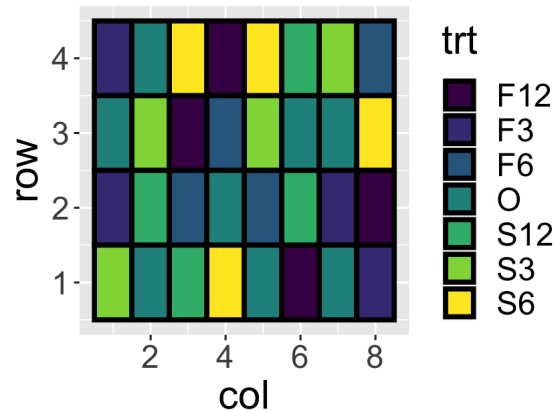
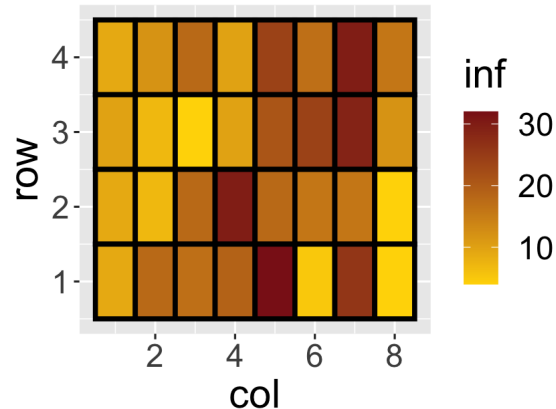
i stacked barplotとpie chartの違いはcoordinate systemが
Cartesian coordinateからpolar coordinateと変わった

🔗 ポテトフィールド研究・このプロットはどうコードする？

```
data(cochran.crd,  
      package = "agridat")
```

cochran.crd

##	inf	trt	row	col
## 1	9	F3	4	1
## 2	12	O	4	2
## 3	18	S6	4	3
## 4	10	F12	4	4
## 5	24	S6	4	5
## 6	17	S12	4	6
## 7	30	S3	4	7
## 8	16	F6	4	8



```
ggplot(cochran.crd,  
       aes(x = col,  
           y = row,  
           fill = inf)) +  
  geom_tile(color = "black", size = 1.2) +  
  scale_fill_gradient(low = "gold",  
                     high = "firebrick4") +  
  theme(text = element_text(size = 20))
```

```
ggplot(cochran.crd,  
       aes(x = col,  
           y = row,  
           fill = trt)) +  
  geom_tile(color = "black", size = 1.2) +  
  scale_fill_viridis_d() +  
  theme(text = element_text(size = 20))
```

2

Grammar of Data Manipulation



Wickham, François, Henry & Müller (2020) dplyr: A Grammar of Data Manipulation. R-package version 1.0.0.

このコードは何をしてる？アウトプットは何を期待しますか？

```
tapply(cochran.crd$inf, cochran.crd$trt, mean)

##      F12      F3      F6      0      S12      S3
##  5.750  9.500 15.500 22.625 14.250 16.750 1

tapply(cochran.crd$inf, cochran.crd$trt, sd)

##      F12      F3      F6      0
## 2.872281 4.932883 3.785939 8.365533 4.

tapply(cochran.crd$inf, cochran.crd$trt,
       function(x) c(avg = mean(x), sd = sd(x))

## $F12
##      avg      sd
## 5.750000 2.872281
##
```

```
library(dplyr)
cochran.crd %>%
  group_by(trt) %>%
  summarise(avg = mean(inf),
            sd = sd(inf))
```

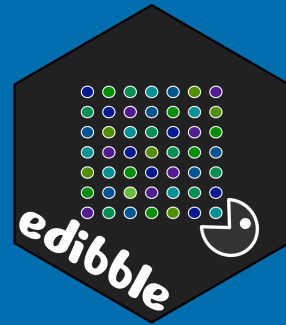
```
## # A tibble: 7 x 3
##   trt      avg      sd
## * <fct> <dbl> <dbl>
## 1 F12      5.75  2.87
## 2 F3       9.5   4.93
## 3 F6      15.5   3.79
## 4 0       22.6   8.37
## 5 S12     14.2   4.86
## 6 S3
## 7 S6
```



右の方が意図が
分かりやすいで
す

3

Grammar of Experimental Design



 Work-In-Progress

実験計画法の一般的なコース

(例えばシドニー大学2017-2019)

教える内容：

- Completely Randomised Design
- Randomised Complete Block Design
- Latin Square Design
- Balanced Incomplete Block Design
- Factorial Design
- ~~2^k Factorial Design~~ (2018年以降取り除いた)
- Split-plot Design (私が2018年に追加した)

Completely Randomised Design (CRD)

- t treatments randomised to n units



observation = mean + treatment + error

(with constraints and distributional assumptions)

ANOVA

Source	df	SS	MS	F	P-value
Treatment	$t - 1$	TSS	MST	$f = \text{MST} / \text{MSR}$	$P(F_{t-1, n-t} > f)$
Residual	$n - t$	RSS	MSR		

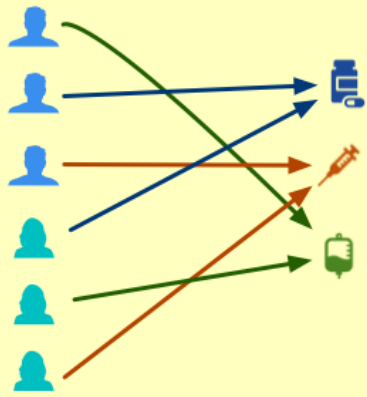
Randomised Complete Block Design (RCBD)

- b blocks of size t
- t treatments randomised to t units within each block

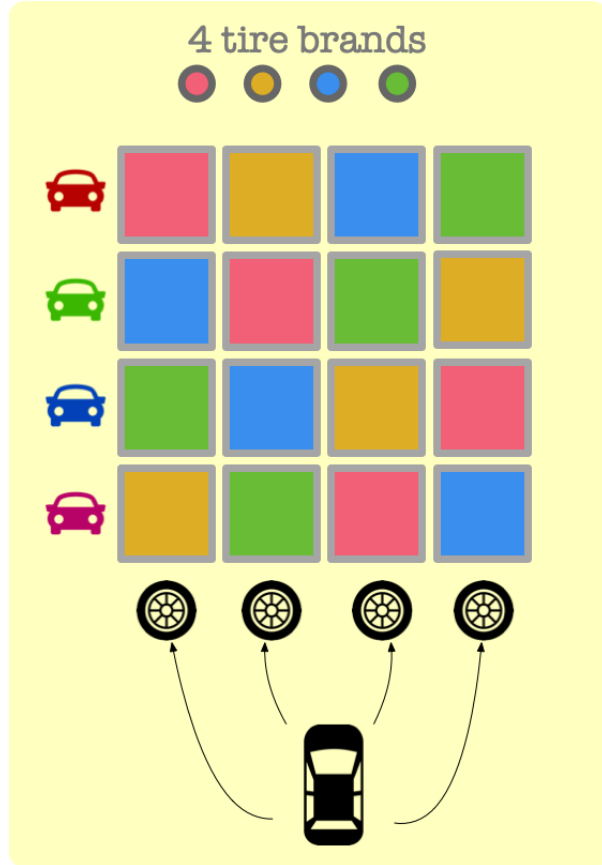
observation = mean + treatment + block + error

ANOVA					
Source	df	SS	MS	F	P-value
Treatment	$t - 1$	TSS	MST	$f = \text{MST} / \text{MSR}$	$P(F_{t-1, (b-1)(t-1)} > f)$
Block	$b - 1$	BSS	MSB		
Residual	$(b - 1)(t - 1)$	RSS	MSR		

6 people 3 types of drugs



Latin Square Design (LSD)

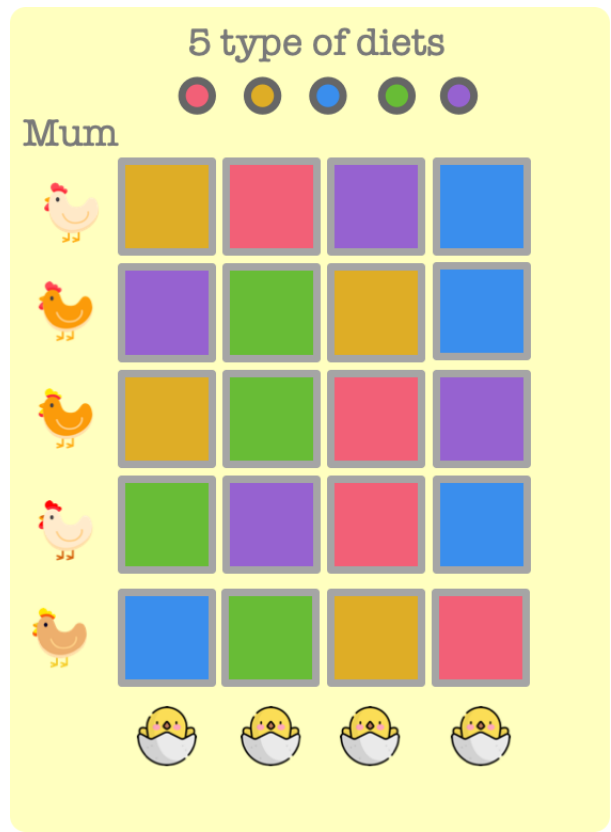


- two orthogonal blocks of size t
- t treatments randomised to units such that every treatment appears exactly once in each block

observation = mean + treatment + row + column + error

ANOVA					
Source	df	SS	MS	F	P-value
Treatment	$t - 1$	TSS	MST	$f = \text{MST} / \text{MSR}$	$P(F_{t-1, (t-2)(t-1)} > f)$
Row	$t - 1$	RowSS	MSRow		
Column	$t - 1$	ColSS	MSCol		
Residual	$(t - 2)(t - 1)$	RSS	MSR		

Balanced Incomplete Block Design (BIBD)



- b blocks of size $k < t$
- t treatments randomised to units within each block such that every pair of treatment appears the same number of times across blocks

$$\text{observation} = \text{mean} + \text{block} + \text{treatment} + \text{error}$$

ANOVA					
Source	df	SS	MS	F	P-value
Block	$b - 1$	BSS	MSB		
Treatment	$t - 1$	TSS Block	MST	$f = \text{MST} / \text{MSR}$	$P(F_{t-1, n-b-t+1} > f)$
Residual	$n - b - t + 1$	RSS	MSR		

Factorial Design

- $ab = t$ treatments randomised to n units
- treatment is every combination of two factors A and B

observation = mean + A + B + A:B + error

ANOVA					
Source	df	SS	MS	F	P-value
Treatment	$ab - 1$	TSS	MST	$f = \text{MST} / \text{MSR}$	$P(F_{ab-1, n-ab} > f)$
Residual	$n - ab$	RSS	MSR		

2 types of fertilizer



4 varieties of carrots



Split-plot Design

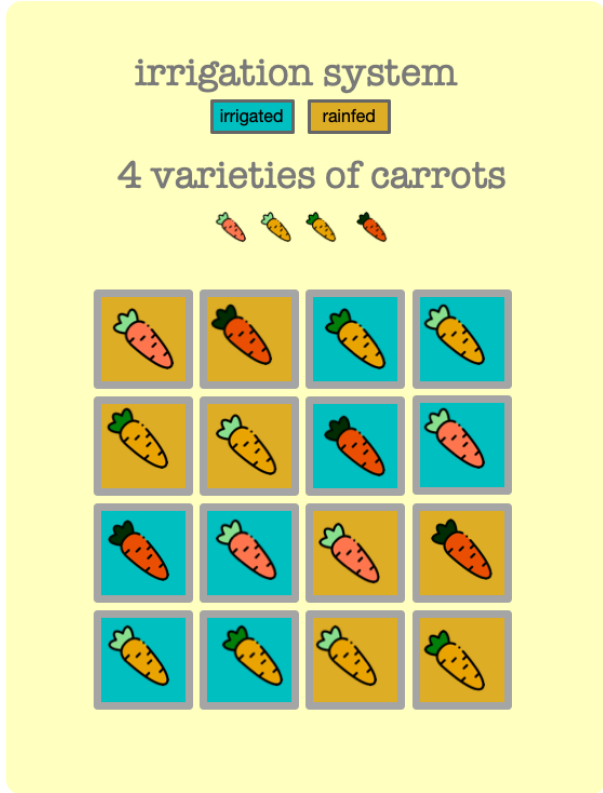
- n_1 whole plots consisting of b sub plots
- in total there are n sub plots
- treatment factor A is randomised to whole plots
- treatment factor B is randomised to sub plots within each whole plot

$$\text{observation} = \text{mean} + A + \text{WP} + B + A:B + \text{error}$$

Not the same
definition as in
sample surveys

ANOVA

Stratum	Source	df	SS	MS	F	P-value
Whole Plot (WP)	Irrigation (A)	$a - 1$	A-SS	MSA		
	WP Residual	$n_1 - a$	WP-SS	MSR-WP		
Sub Plot (SP)	Variety (B)	$b - 1$	B-SS	MSB		
	A:B	$(a - 1)(b - 1)$	AB-SS	MSAB	$f^* = \text{MSAB} / \text{MSR-SP}$	$P(F_{(a-1)(b-1), n-ab-n_1+a} > f^*)$
	SP Residual	$n - ab - (n_1 - a)$	SP-RSS	MSR-SP		



CRAN Task View of Design of Experiments

contains

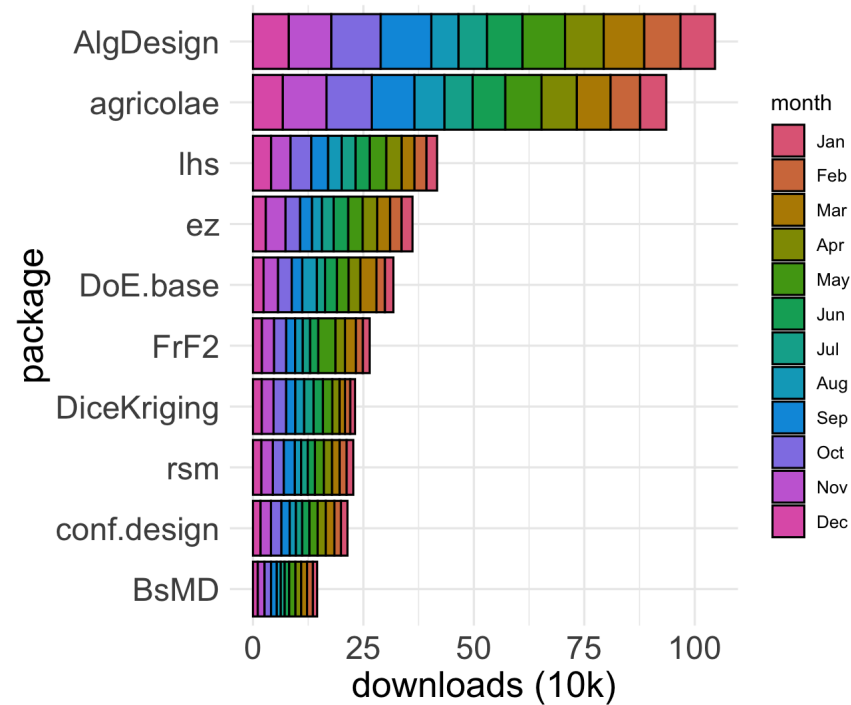


224 R-packages

as of 2021-01-21

(Please note that there may be some webscrapping error)

ダウンロードされたR-packages トップ 10



AlgDesign and **agricolae** are the most downloaded

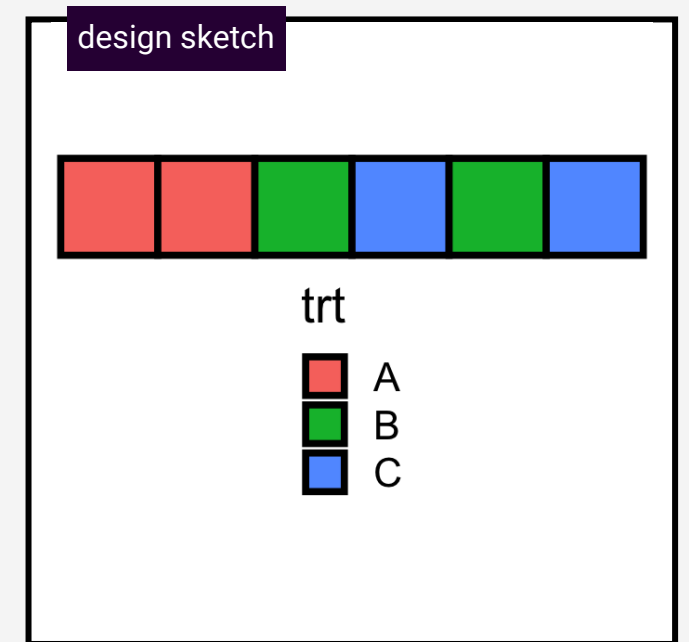
(data from [cranlogs](https://cranlogs.r-pkg.org/) from 2015-01-01 to 2020-12-31)

agricolae::design.crd

Completely randomised design for $t = 3$ treatments with 2 replicates each

```
trt <- c("A", "B", "C")
agricolae::design.crd(trt = trt, r = 2) %>% glimpse()
```

```
## List of 2
## $ parameters:List of 7
## ..$ design: chr "crd"
## ..$ trt : chr [1:3] "A" "B" "C"
## ..$ r : num [1:3] 2 2 2
## ..$ serie : num 2
## ..$ seed : int 2074805913
## ..$ kinds : chr "Super-Duper"
## ..$ : logi TRUE
## $ block : data frame with 6 obs of 2 variables:
```

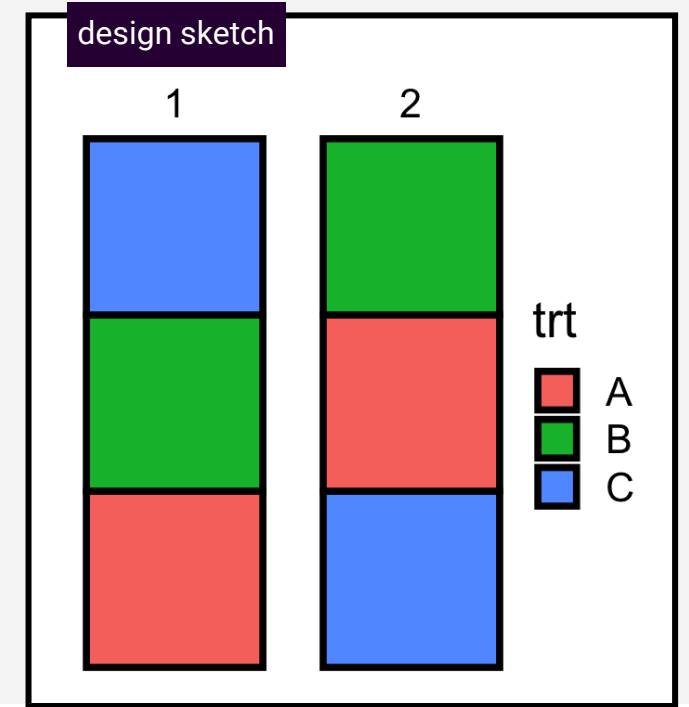


agricolae::design.rcbd

Randomised complete block design for $t = 3$ treatments with 2 blocks

```
trt <- c("A", "B", "C")
agricolae::design.rcbd(trt = trt, r = 2) %>% glimpse()
```

```
## List of 3
## $ parameters:List of 7
## ..$ design: chr "rcbd"
## ..$ trt : chr [1:3] "A" "B" "C"
## ..$ r : num 2
## ..$ serie : num 2
## ..$ seed : int 490734433
## ..$ kinds : chr "Super-Duper"
## ..$ : logi TRUE
## $ sketch : chr [1:2] "A" "C" "B" "A"
```

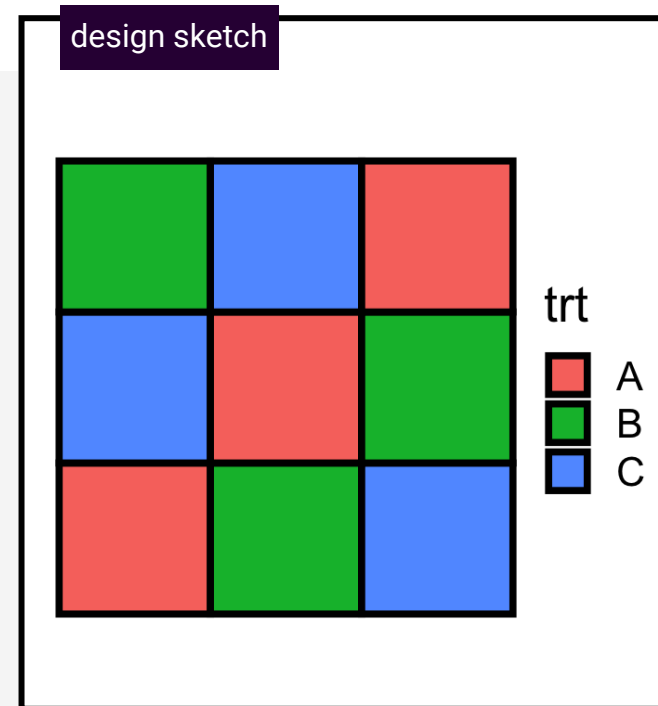


agricolae::design.lsd()

Latin square design for $t = 3$ treatments

```
trt <- c("A", "B", "C")
agricolae::design.lsd(trt = trt) %>% glimpse()

## List of 3
## $ parameters:List of 7
## ..$ design: chr "lsd"
## ..$ trt : chr [1:3] "A" "B" "C"
## ..$ r : int 3
## ..$ serie : num 2
## ..$ seed : int -338489375
## ..$ kinds : chr "Super-Duper"
## ..$ : logi TRUE
## $ sketch : chr [1:3] "A" "B" "C"
```

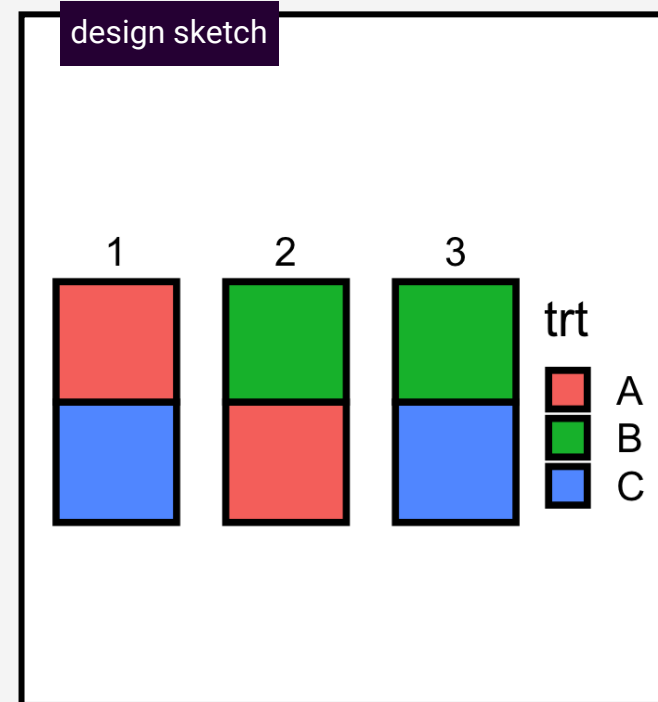


agricolae::design.bib()

Balanced incomplete block design for $t = 3$ treatments with block size of 2

```
trt <- c("A", "B", "C")
agricolae::design.bib(trt = trt, k = 2) %>% glimpse()

## [1] "No improvement over initial random design."
##
## Parameters BIB
## =====
## Lambda      : 1
## treatmeans  : 3
## Block size  : 2
## Blocks      : 3
## Replication: 2
##
```



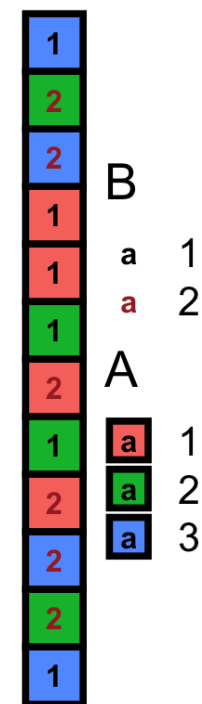
agricolae::design.ab()

Factorial design for $t = 3 \times 2$ treatments with 2 replication for each treatment

```
agricolae::design.ab(trt = c(3, 2), r = 2, design = "crd") %>% glimpse()
```

```
## List of 2
## $ parameters:List of 8
## ..$ design : chr "factorial"
## ..$ trt     : chr [1:6] "1 1" "1 2" "2 1" "2 2" ...
## ..$ r      : num [1:6] 2 2 2 2 2 2
## ..$ serie  : num 2
## ..$ seed   : int -751356955
## ..$ kinds  : chr "Super-Duper"
## ..$       : logi TRUE
## ..$ applied: chr "crd"
```

design sketch



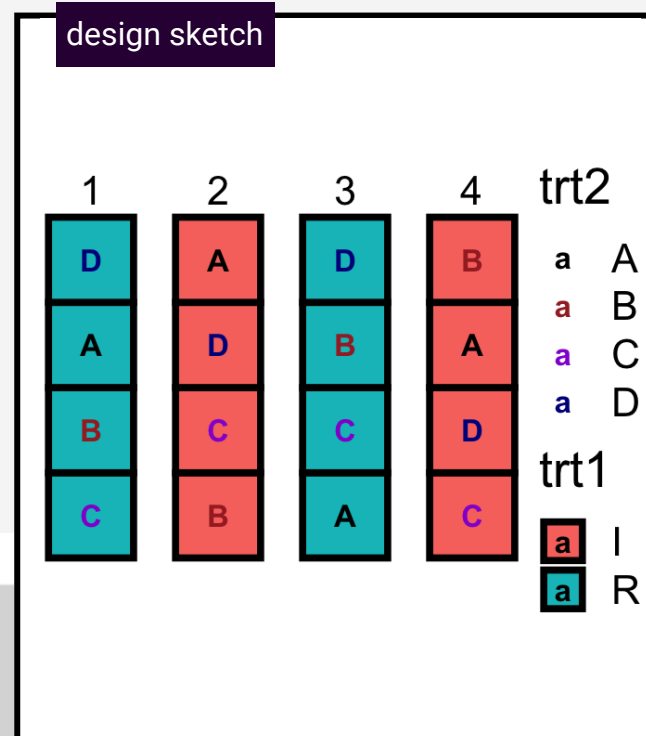
Note *not* A/B testing!

agricolae::design.split()

Split-plot design for $t = 2 \times 4$ treatments with 2 replication for each treatment

```
trt1 <- c("I", "R"); trt2 <- LETTERS[1:4]
agricolae::design.split(trt1 = trt1, trt2 = trt2, r = 2, design = "crd") %>%
  glimpse()
```

```
## List of 2
## $ parameters:List of 8
## ..$ design : chr "split"
## ..$       : logi TRUE
## ..$ trt1    : chr [1:2] "I" "R"
## ..$ applied: chr "crd"
## ..$ r      : num [1:2] 2 2
## ..$ serie  : num 2
```

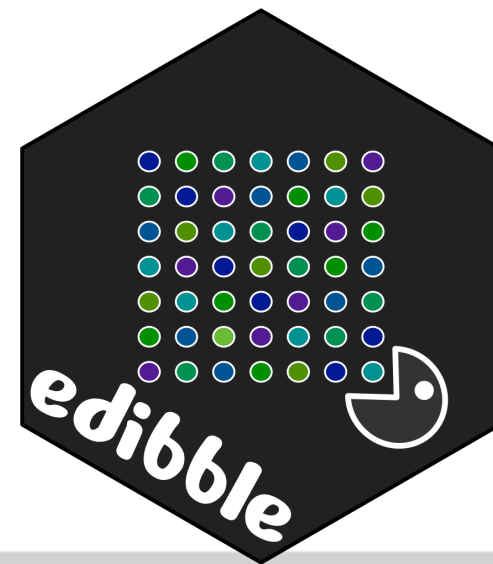


実験計画法の文法とは

- Base R プロット覚えてますか？ ▶ [base plot](#)
- 🤔 "named experimental design" functions ([agricolae::design.crd](#), etc.) are like "named statistical graphic" functions ([pie](#), [barplot](#))
- 💡🔧 このコンセプトが [edibble](#) R-packageのもとです
<https://github.com/emitanaka/edibble>

名前の元

- [tibble](#) R-package とは modern reimagining of the [data.frame](#)
- [edibble](#) とは **e**xperimental **d**esign **tibble**



edibble プロトタイプ

- Consider a field experiment with 32 plots
- There are 7 different treatments
- Allocate treatments to plots
- Randomise treatments to plots
- The result is a **completely randomised design**

```
library(edibble)
start_design(name = "cochran.crd") %>%
  set_units(plot = 32) %>%
  set_trts(trt = c("F12", "F3", "F6", "0",
                  "S12", "S3", "S6")) %>%
  allocate_trts(~ plot) %>%
  randomise_trts() %>%
  serve_table()
```

```
## # An edibble: 32 x 2
##   plot      trt
##   <unit(32)> <trt(7)>
## 1 plot1     F12
## 2 plot2     S6
## 3 plot3     F6
## 4 plot4     0
## 5 plot5     S6
```

edibble プロトタイプ

- Consider a field experiment with 2 blocks each with 16 plots
- There are 7 different treatments
- Allocate treatments to plots
- Randomise treatments to plots within blocks
- Resulting design is a **randomised block design**

前の実験研究法とどう違うか分かりますか？

```
library(edibble)
start_design(name = "cochran.crd") %>%
  set_units(block = c("B1", "B2"),
            plot = nested_in(block, 16)) %>%
  set_trts(trt = c("F12", "F3", "F6", "0",
                  "S12", "S3", "S6")) %>%
  allocate_trts(~ plot) %>%
  randomise_trts() %>%
  serve_table()
```

```
## # An edibble: 32 x 3
##   block      plot      trt
##   <unit(2)> <unit(32)> <trt(7)>
## 1 B1      plot1      S6
## 2 B1      plot2      S3
## 3 B1      plot3      F12
## 4 B1      plot4      F6
```

edibble ユニット・ストラクチャー

```
start_design("complex unit structure") %>%  
  set_units(city = c("tokyo", "nagano", "sydney", "melbourne", "washington"),  
            school = nested_in(city,  
                                "tokyo" ~ 4,  
                                "sydney" ~ 1,  
                                . ~ 2)) %>%
```

```
serve_table()
```

```
## # An edibble: 11 x 2  
##   city      school  
##   <unit(5)> <unit(11)>  
## 1 tokyo    school1  
## 2 tokyo    school2  
## 3 tokyo    school3  
## 4 tokyo    school4
```


edibble トリートメント・ストラクチャー

```
des <- start_design(name = "Effective teaching") %>%
  set_units(class = 4,
            student = nested_in(class, 30)) %>%
  set_trts(style = c("flipped", "traditional"),
          exam = c("take-home", "open-book", "closed-book")) %>%
  allocate_trts(style ~ class,
               exam ~ student) %>%
  randomise_trts()

print(serve_table(des), n = 120)

## # An edibble: 120 x 4
##      class      student      style      exam
##      <unit(4)> <unit(120)> <trt(2)>    <trt(3)>
##  1 class1      student1    flipped    closed-book
```

Recording variables in **edibble** • 記録

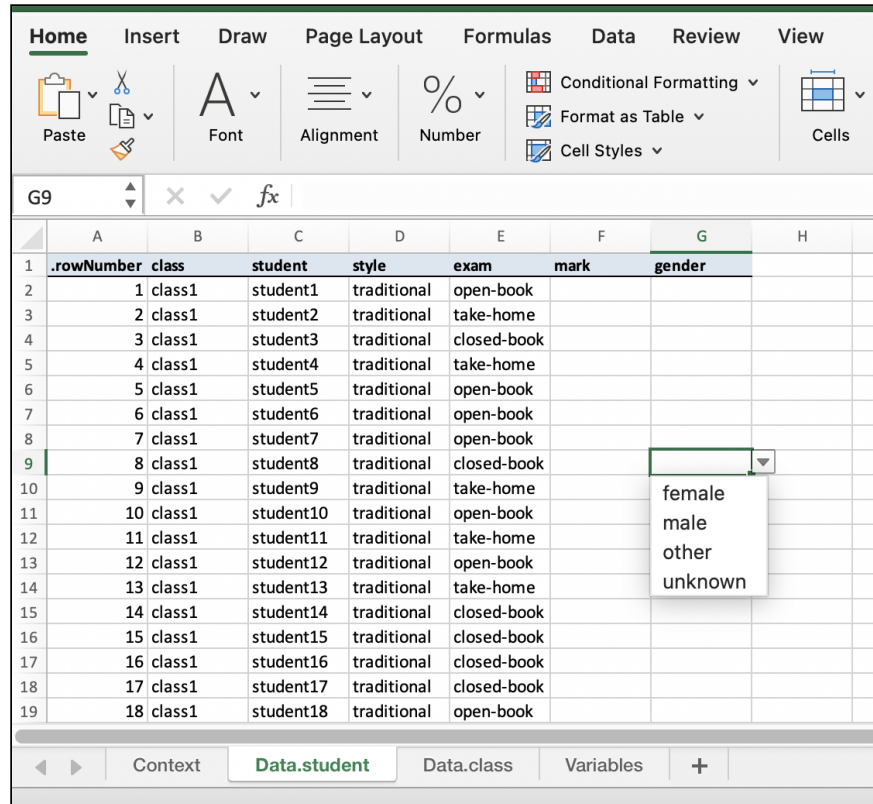
```
out <- des %>%  
  record_vars(student = c(mark, gender),  
              class = teacher) %>%  
  expect_vars(mark = to_be_numeric(with_value(between = c(0, 100))),  
             gender = to_be_factor(levels = c("female", "male", "other", "unknown"))) %>%  
  serve_table()
```

out

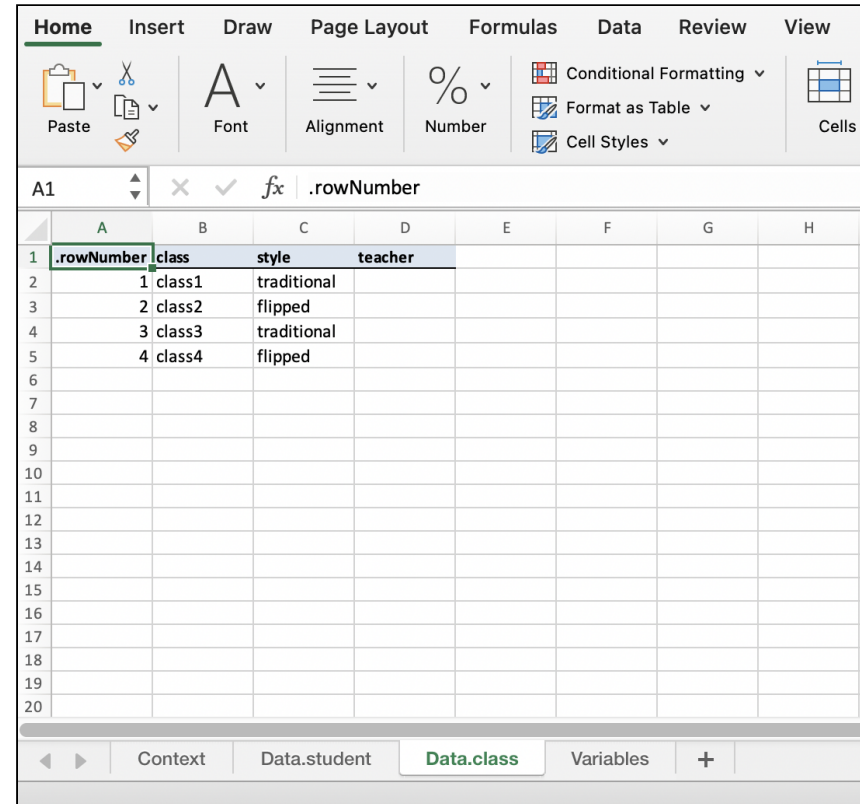
```
## # An edibble: 120 x 7  
##   class      student      style      exam      mark gender teacher  
##   <unit(4)> <unit(120)> <trt(2)> <trt(3)>   <rcrd> <rcrd> <rcrd>  
## 1 class1     student1     flipped closed-book  ■      ■      ■  
## 2 class1     student2     flipped closed-book  ■      ■      x  
## 3 class1     student3     flipped open-book   ■      ■      x  
## 4 class1     student4     flipped open-book   ■      ■      x  
## 5 class1     student5     flipped open-book   ■      ■      x
```

edibble アウトプット

```
export_design(out, file = "design.xlsx")
```



	A	B	C	D	E	F	G	H
1	.rowNumber	class	student	style	exam	mark	gender	
2	1	class1	student1	traditional	open-book			
3	2	class1	student2	traditional	take-home			
4	3	class1	student3	traditional	closed-book			
5	4	class1	student4	traditional	take-home			
6	5	class1	student5	traditional	open-book			
7	6	class1	student6	traditional	open-book			
8	7	class1	student7	traditional	open-book			
9	8	class1	student8	traditional	closed-book			
10	9	class1	student9	traditional	take-home			
11	10	class1	student10	traditional	open-book			
12	11	class1	student11	traditional	take-home			
13	12	class1	student12	traditional	open-book			
14	13	class1	student13	traditional	take-home			
15	14	class1	student14	traditional	closed-book			
16	15	class1	student15	traditional	closed-book			
17	16	class1	student16	traditional	closed-book			
18	17	class1	student17	traditional	closed-book			
19	18	class1	student18	traditional	open-book			



	A	B	C	D	E	F	G	H
1	.rowNumber	class	style	teacher				
2	1	class1	traditional					
3	2	class2	flipped					
4	3	class3	traditional					
5	4	class4	flipped					
6								
7								
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20								

実験計画は重要です!

edibbleの目的は実験計画を容易にする事です

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コメントとフィードバックを歓迎します！

This slide is made using the [xaringan](#) R-package and found at

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Thank you!

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