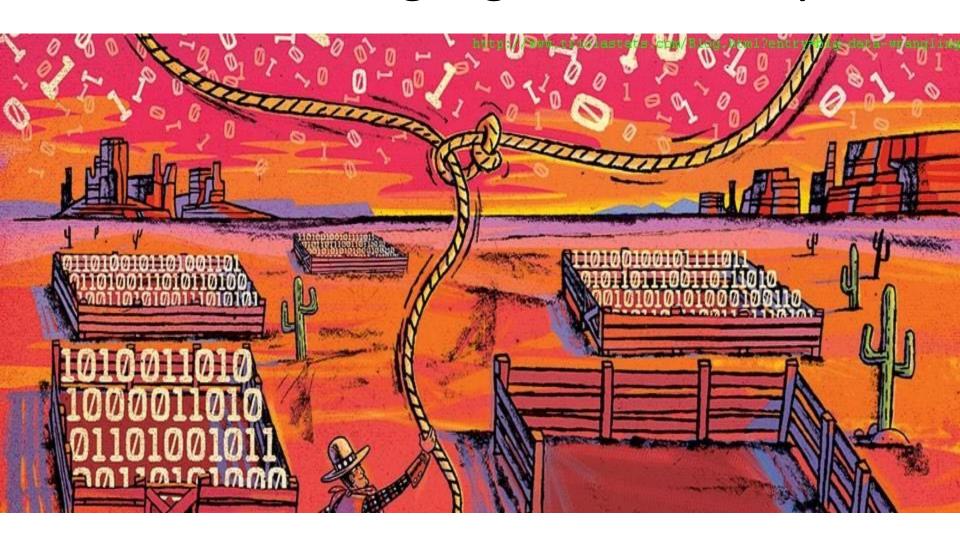
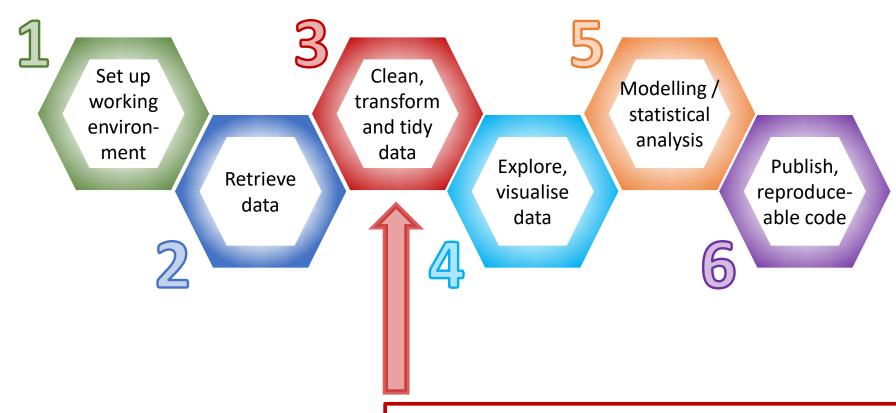
Palaeodata wrangling with the Tidyverse







Palaeodata Workflow



Based on Fig 3, Slater et al. 2019. Using R in hydrology: a review of recent developments and future directions. Hydrology and Earth System Sciences 23:2939-2963.

Not sexy, not clever, not always straightforward, and can be very time consuming.

Having a good set of tools in R can:

- Increase efficiency
- Reduce errors
- Self-documenting & reproducible

Guiding principles

- **Everything** is possible in **Base R** but solutions may be ad-hoc and need a mix functions & packages with different syntax: the Wild West that is Base R!
- **Tidyverse** offers a consistent approach to data wrangling, fast, concise & logical syntax, and very flexible.
- Some things may be faster in Base R but speed is rarely a limiting factor.
- Focus on code that is simple, readable and easy to understand (promote learning, easier debugging, and reproducibility).
- Today don't get bogged down in the details of individual functions and operations. Focus on the big picture - the details will come with practice.

Resources

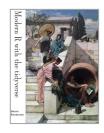
Whickham & Grolemund, R for Data Science, free online https://r4ds.had.co.nz/



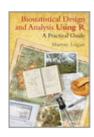
Locke, R Fundamentals 2: Data Manipulation (£11) https://itsalocke.com/company/books/



Bruno Rodrigues, Modern R with the tidyverse free online https://b-rodrigues.github.io/modern R/ or buy pdf for < £10



Murray Logan's website, excellent tutorials & book https://www.flutterbys.com.au/stats/



Rstudio cheatsheets

https://www.rstudio.com/resources/cheatsheets/

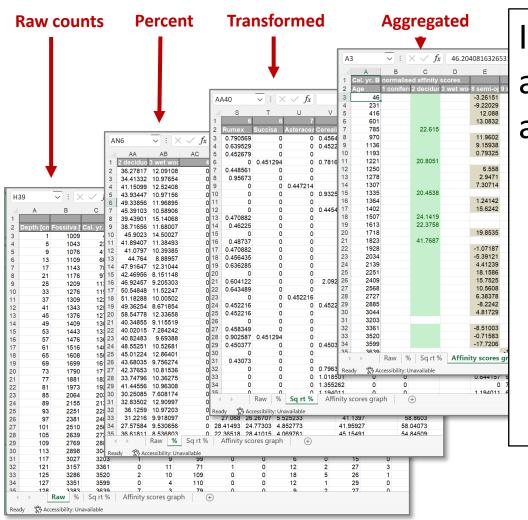


stackoverflow + 1001 other websites...



Do you need the tidyverse?

Do you have many separate files / sheets of the same data? (counts, percentages, subsets, aggregated)



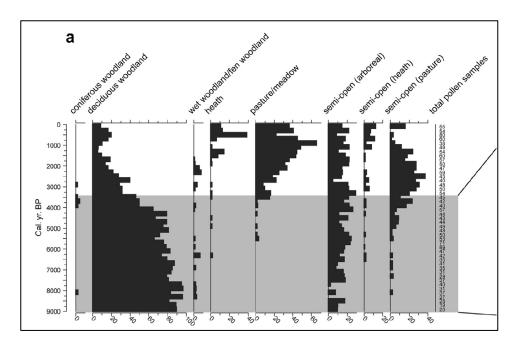
If yes, then you should aim to have only one file and do all processing in R.

- More efficient (fewer files to keep track of)
- Reduces errors (and easier to correct errors and update data – only 1 file to change)
- Reproducible (record of what you did and why)

Example: Impact of the Neolithic Agricultural Transition

Jessie Woodbridge, Ralph Fyfe & colleagues Woodbridge et al. (2014) & Fyfe et al. (2010)

Aim: Reconstruct anthropogenic land-cover change in Britain over the last 9000 years



Land-cover reconstructions for Britain Figure 3 from Woodbridge et al. (2014)



Fyfe, et al. 2010. A pollen-based pseudobiomisation approach to anthropogenic land-cover change. The Holocene **20:1165-1171.**

Woodbridge, et al. 2014. The impact of the Neolithic agricultural transition in Britain: a comparison of pollenbased land-cover and archaeological 14C date-inferpoll population change. Journal of Archaeological Science 51:216-224.

Thanks to Jessie
Woodbridge and
Ralph Fyfe for
sharing their data!

Day 1 aims

Morning

Aims: To reproduce Woodbridge et al. Figure 3 using Tidyverse methods & explore changes in palynological richness.

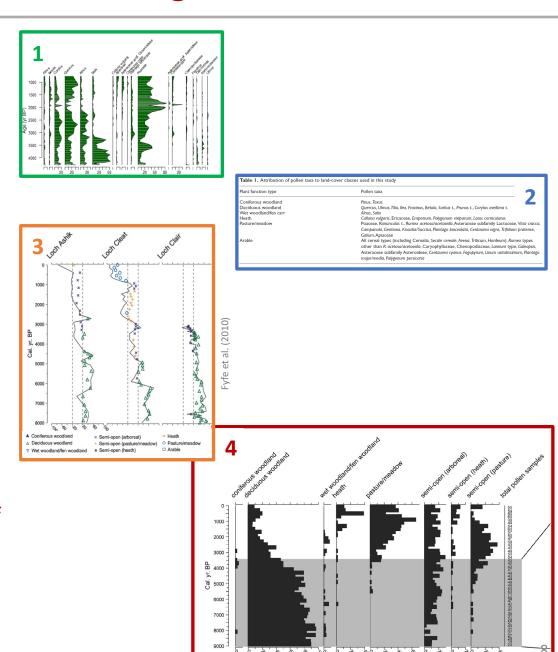
- 1. Work through analysis of a single site using base R
- 2. Repeat using Tidyverse
- 3. Apply to all (41) sites & create synthesis figure
- 4. Modelling species richness with the Tidyverse

Afternoon

- Demonstration of my new package riojaPlot for plotting stratigraphic diagrams
- Work with your own data, ask questions, get help

Example: Impact of the Neolithic Agricultural Transition

- 1. Extract dated pollen profiles from European pollen database (+ other sources), 41 sites in total.
- 2. Classify each pollen type to a land cover class (LCC)
- 3. For each site, transform species data to major vegetation types (land cover class: LCC) and calculate the dominant LCC for each sample.
- 4. Sum dominant LCCs for all sites in 200 year time slices, convert to % of each LCC & plot.

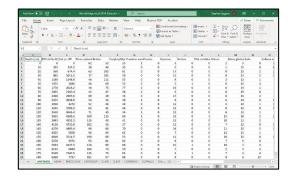


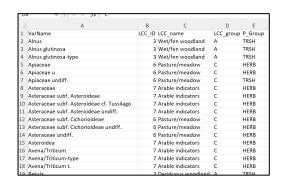
The data

- 1. Woodbridge_et_al_2014_Data.xlsx: Excel file with pollen counts for 42 sites, each site on a separate tab. Columns for pollen types, Depth and Cal. Age BP + alternative chronologies, sample IDs & and pollen sum.
- **2.** LCC_Info.xlsx: Excel file with the following worksheets:

LCC_lookup: Lookup table of taxon names and corresponding land cover classes.

Site_info: Information about each site, including region, grid references etc.





Site_no	Site_code	Site_name	Region	Region2	Longit	atitud	Site_t	Reference
1	ANFSHEIL	Allt na Feithe	East Scotland	Scotland	-3.7	56.23	Bog	Birks, H.H. 19
21	ASHIK	Loch Ashik	North Scotla	Scotland	-5.8	57.25	Small	Birks, H.J.B.,
2	BREDCOUN	Brede Bridge	Southeast Er	England	-0.6	50.93	Medi	Waller, M.P.
5	CHROISGP	Loch a'Chrois	North Scotla	Scotland	-5.3	57.57	Medi	Pennington, \
26	CLAIR	Loch Clair	North Scotla	Scotland	-5.3	57.56	Large	Waller, M.P.

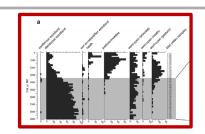
Land Cover Classification (LCC) method

Step1: Calculate LCC for each site

- 1. Import data
- 2. Clean data remove unwanted columns
- 3. Rename columns
- 4. Convert counts to percentages
- 5. Allocate each pollen type to an LCC class and sum sqrt-percentages across each class
- 6. Normalise the sqrt-percent LCC data to 100%
- 7. Identify the dominant LCC class at each level

Step2: Aggregate multiple sites

- 8. Aggregate data from all sites and count the number of levels in each LCC class in 200 year time slices (N)
- 9. Convert N to percentage of each LCC class in each time slice
- 10. Plot the aggregated data

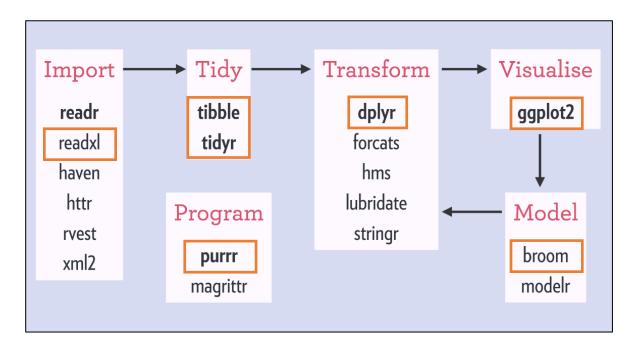


Part 1: Code Step 1 in Base R

Palaeodata wrangling with the tidyverse

What is the Tidyverse?

- Collection of R packages designed for data science that share common interface standards, grammar and data structures
- You spend more time on concepts and less sorting out syntax
- Promotes code readability



 Both general purpose packages: tibble for data frames, tidyr for tidying, dplyr for transforming and ggplot for visualisation, and specialised packages for data import (readxl), dates & time (lubridate, hms), strings (stringr), factors (forcats) plus others.

Core features

1. Uses tibbles rather than data frames

```
refined print method strict about $ subsetting, doesn't like rownames easier to created nested data frames
```

2. Encourages use of the pipe %>%

```
Instead of summary(lm(y~x, data=df))
Use df %>% lm(y~x, data=.) %>% summary()
```

3. Promotes use of tidy data

Every column is a variable Every row is an observation Every cell is a single value

Tidy data

Not tidy!

(because the variable is pollen type and the attributes are taxon and count)

Depth (cm)	Cal. yr. BP	Pinus sylve	Taxus bac	Betula	Betula/Co
132	1514	3	1	40	2
164	1618.5	3	3	33	1
196	1723	3	2	34	2
228	1827.5	4	4	33	1
260	1932	5	3	34	3
268	2143.75	4	3	43	0
276	2355.5	14	2	40	0
284	2567.25	11	1	60	0
292	2779	10	3	54	2



Tidy!

(Each column is a variable, pollen counts are described by key/value pairs)

Depth (cm)	Cal. yr. BP	Taxon	Count
132	1514	Pinus sylvestris	3
132	1514	Taxus baccata	1
132	1514	Betula	40
132	1514	Betula/Corylus/Myrica	2
164	1618.5	Pinus sylvestris	3
164	1618.5	Taxus baccata	3
164	1618.5	Betula	33
164	1618.5	Betula/Corylus/Myrica	1
196	1723	Pinus sylvestris	3

Wide format

Convert from wide to long with

```
pivot_longer()

df %>% pivot_longer(
   cols=-c(`Depth (cm)`, `Cal. yr. BP`),
   names to="Taxon", values to="Count")
```

Long format

pivot wider()

Convert from long to wide with

```
df %>% pivot_wider(
  id_cols=c(`Depth (cm)`, `Cal. yr. BP`),
  names from=Taxon, values from=Count)
```

In package tidyr

dplyr functions for data transformation

```
dplyr function
select: select columns (subset)
                                                         Base R equivalent
filter: subsetting rows based on condition (subset)
arrange: sorting (sort, order)
distinct: find unique values (unique)
slice: selecting rows based on position ([])
mutate: create new columns (transform)
group by: defining groups of rows to process subsets
summarise: summarise data (optionally by group) (aggregate)
*_join: merging data sets (merge)
bind_rows, bind_cols: combine multiple dfs by row or column
                                                     (rbind, cbind)
```

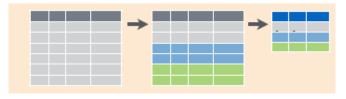
Creating new variables using mutate



Depth (cm)	Cal. yr. BP	Taxon	Count
132	1514	Pinus sylvestris	3
132	1514	Taxus baccata	1
132	1514	Betula	40
132	1514	Betula/Corylus/Myrica	2
164	1618.5	Pinus sylvestris	3
164	1618.5	Taxus baccata	3
164	1618.5	Betula	33
164	1618.5	Betula/Corylus/Myrica	1
196	1723	Pinus sylvestris	3

d	f %>%				
	mutate(SQRT Cou	nt=sqrt(Count))	
A	tibble: 9 x 5	_			
	`Depth (cm)`	`Cal. yr. BP`	Taxon	Count	SQRT_Count
	<dbl></dbl>	<db1></db1>	<chr></chr>	<db1></db1>	_ <dbl></dbl>
1	132	1514	Pinus sylvestris	3	1.73
2	132	1514	Taxus baccata	1	1
3	132	1514	Betula	40	6.32
4	132	1514	Betula/Corylus/Myrica	2	1.41
5	164	1618.	Pinus sylvestris	3	1.73
6	164	1618.	Taxus baccata	3	1.73
7	164	1618.	Betula	33	5.74
3	164	1618.	Betula/Corylus/Myrica	1	1
9	196	1723	Pinus sylvestris	3	1.73

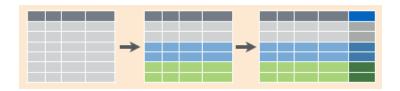
Summarising by group



Split -> Apply -> Combine

Depth (cm)	Cal. yr. BP	Taxon	Count
132	1514	Pinus sylvestris	3
132	1514	Taxus baccata	1
132	1514	Betula	40
132	1514	Betula/Corylus/Myrica	2
164	1618.5	Pinus sylvestris	3
164	1618.5	Taxus baccata	3
164	1618.5	Betula	33
164	1618.5	Betula/Corylus/Myrica	1
196	1723	Pinus sylvestris	3

Compute new variables by group



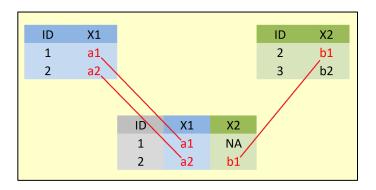
Depth (cm)	Cal. yr. BP	Taxon	Count
132	1514	Pinus sylvestris	3
132	1514	Taxus baccata	1
132	1514	Betula	40
132	1514	Betula/Corylus/Myrica	2
164	1618.5	Pinus sylvestris	3
164	1618.5	Taxus baccata	3
164	1618.5	Betula	33
164	1618.5	Betula/Corylus/Myrica	1
196	1723	Pinus sylvestris	3

```
df %>%
    group by (`Depth (cm)`) %>%
    mutate(Percent=Count/sum(Count)*100)
`Depth (cm)` `Cal. yr. BP` Taxon
                                             Count Percent
        <db1>
                     <dbl> <chr>
                                               <db1>
                                                       <db1>
                                                        6.52
          132
                     1514 Pinus sylvestris
          132
                     1514
                           Taxus baccata
                                                   1
                                                        2.17
          132
                     1514 Betula
                                                  40
                                                       87.0
          132
                     1514 Betula/Corylus/Myrica
                                                        4.35
                     1618. Pinus sylvestris
          164
                                                        7.5
6
                                                        7.5
          164
                     1618. Taxus baccata
          164
                     1618. Betula
                                                  33
                                                       82.5
                     1618. Betula/Corylus/Myrica
          164
                                                        2.5
9
                     1723 Pinus sylvestris
                                                   3 100
          196
```

Merging tables

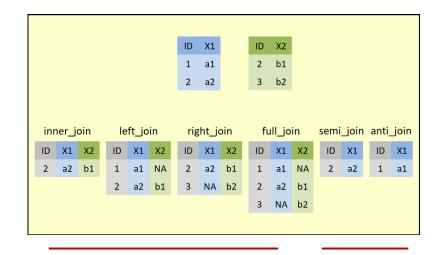
Join or merge tables using column(s) common to both tables

Left join – all rows from left df, matching rows from right



Df1 %>% left join(df2, by='ID')

Other join types



Mutating joins: combine variables from the 2 sources

Filtering joins: use right hand df to filter rows in lh df

Working across rows using across ()

Depth (cm)	Cal. yr. BP	Pinus sylve	Taxus bac	Betula	Betula/Co
132	1514	3	1	40	2
164	1618.5	3	3	33	1
196	1723	3	2	34	2
228	1827.5	4	4	33	1
260	1932	5	3	34	3
268	2143.75	4	3	43	
276	2355.5	14	2	40	
284	2567.25	11	1	60	
292		10	3	54	2

```
# Base R replace in situ
df[is.na(df)] <- 0
# Base R create new df
replace(df, is.na(df), 0)
# Tidyverse, replace NAs in a single column
df %>% mutate(Betula = replace na(Betula, 0)))
```

Use across() to select, rename, or apply a transformation to multiple columns

```
across(.cols = everything(), .fns = NULL, ..., .names = NULL)
.cols = columns to transform
.fns = function to apply to each column
.names = how the new columns will be names (default is to use original names)
# Tidyverse, replace NAs except in cols 1 & 2
df %>% mutate(across(-(1:2), ~replace na(.x, 0)))
```

Part 2: Code it using the Tidyverse

Code comparison: Part 1

Base R

```
polldata <- read_excel("Woodbridge_et_al_2014_Data.xlsx",</pre>
sheet="REDMERE")
lcc_lookup <- read_excel("LCC_info.xlsx", sheet="LCC_Lookup")</pre>
1cc lookup
non_pollen <- c("Sample", "Radiocarbon years B.P.", "EPD default
[yrs.BP.]", "EPD [yrs.BP.]", "Fossilva [yrs.BP.]", "Sum")
del <- colnames(polldata) %in% non_pollen</pre>
polldata <- polldata[, !del]</pre>
depth_age <- subset(polldata, select=c(`Depth (cm)`, `Cal. yr. BP`))</pre>
poll_count <- subset(polldata, select=-c(`Depth (cm)`, `Cal. yr. BP`))</pre>
colnames(depth_age) <- c("Depth", "Age_BP")</pre>
poll_pc <- poll_count / rowSums(poll_count) * 100</pre>
poll sart <- sart(poll pc)</pre>
sel <- match(colnames(poll_sqrt), lcc_lookup$varName)</pre>
taxa_lcc <- lcc_lookup[sel, ]
poll_lcc <- t (rowsum(t(poll_sqrt), group=taxa_lcc$LCC_name))</pre>
poll_lcc <- data.frame(poll_lcc, check.names=FALSE)</pre>
poll_norm <- poll_lcc / rowSums(poll_lcc) * 100</pre>
dominant_class <- apply(poll_norm, 1, which.max)</pre>
poll_norm$lcc_class <- factor(colnames(poll_norm)[dominant_class])</pre>
sum_arboreal <- rowSums(poll_norm[, c("Coniferous woodland",</pre>
                                        "Deciduous woodland",
                                        "Wet/fen woodland")]) # arboreal
sum_open <- rowSums(poll_norm[, c("Heath",</pre>
                                        "Pasture/meadow",
                                        "Arable indicators")]) # open
poll_norm$Affinity <- sum_arboreal - sum_open</pre>
plot(depth_age$Age_BP, poll_norm$Affinity, type="l",
     xlab="Age (years BP)",
     ylab="Affinity")
points(depth_age$Age_BP, poll_norm$Affinity, pch=19, cex=1,
col=as.integer(poll norm$lcc class))
legend("topleft". pch=19. col=1:7. legend=levels(poll norm$lcc class))
```

Tidyverse

```
polltidy <- read_excel("Woodbridge_et_al_2014_Data.xlsx", sheet="REDMERE")</pre>
lcc_lookup <- read_excel("LCC_info.xlsx", sheet="LCC_Lookup")</pre>
non_pollen <- c("Sample","Radiocarbon years B.P.", "EPD default [yrs.BP.]",</pre>
"EPD [yrs.BP.]", "Fossilva [yrs.BP.]", "Sum")
polltidy_long <- polldata %>%
  rename("Depth"= Depth (cm) , "Age_BP"= Cal. yr. BP ) %>%
pivot_longer(cols=-c("Depth", "Age_BP"),
               names_to="VarName", values_to="Count") %>%
  filter(!(VarName %in% non_pollen))
polltidy_sqrt <- polldata_long %>%
  group_by(Depth) %>%
  mutate(Percent = Count / sum(Count) * 100,
         SORT PC = sqrt(Percent)) %>%
  ungroup()
polltidy_norm <- polltidy_sqrt %>%
  left_join(lcc_lookup, by="varName") %>%
  group_by(Depth, Age_BP, LCC_name, LCC_group) %>%
  summarise(SQRT_PC=sum(SQRT_PC), .groups="drop") %>%
  group by(Depth. Age BP) %>%
  mutate(Norm_SQRT_PC=SQRT_PC/sum(SQRT_PC)*100) %>%
  ungroup() %>%
  select(-SQRT_PC)
polltidy_lcc <- polltidy_norm %>%
  group_by(Depth, Age_BP) %>%
  mutate(A=sum(Norm_SQRT_PC[LCC_group=="A"]),
         C=sum(Norm_SQRT_PC[LCC_group=="C"]),
         Affinity=A-C) %>%
  select(-c(A, C)) %>%
  slice_max(Norm_SQRT_PC, n=1, with_ties=FALSE) %>%
  select(-c(Norm_SQRT_PC)) %>%
  ungroup()
ggplot(polltidy_lcc, aes(x=Age_BP, y=Affinity, col=LCC_name)) +
  geom_line(col="grey") +
  geom point(size=2) +
  scale_x_continuous(breaks=seg(0, 10000, by=500)) +
  labs(x="Years BP") +
  scale_colour_discrete(name="LCC") +
  theme(legend.position="top") +
  guides(col=guide_legend(nrow=2))
```

Working with multiple datasets – base R

How to apply our LCC code for 1 site to many? Use a for loop!

```
for (val in sequence) {
    statement
}

sequence is a vector and val takes on each
of its values during the loop. In each iteration
statement is evaluated.
```

```
x <- 1:5
for (i in x) {
   print(i)
}
[1] 1
[1] 2
[1] 3
[1] 4
[1] 5</pre>
```

Rewriting code as a function

- To apply our LCC function to multiple sites we can use a loop and collate results at each iteration.
- We could include all the LCC code within the loop but this
 is not good makes the code more complex, and we
 should aim to reuse code, not repeat it.
- Encapsulate the code in a function, and call the function from within the loop.

```
Defining a function:

my_fun <- function(arg1, arg2, ...) {
    statements
    return(object)
}</pre>
```

```
Example:

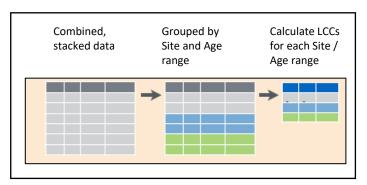
my_fun <- function(a, b) {
   c <- a + b
   return(c)
}
my_fun(2, 3)
[1] 5</pre>
```

Part 3: Code to aggregate multiple sites Base R

Working with multiple datasets – Tidyverse

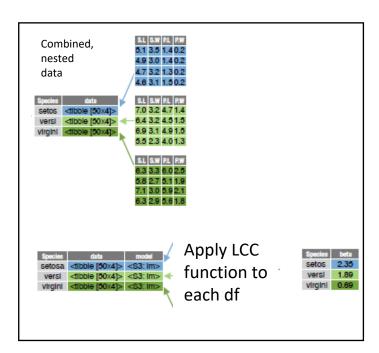
Two approaches with Tidy functions that avoid loops and produce more readable, elegant code:

1. Convert each df to long format, and stack, and perform summaries / transformations by grouping of Site and Age/Depth



2. Convert to nested data frame that stores data of each site within the cell of a larger organising table. Apply a function to each nested table and collate results.

We use second approach to clean data and convert to long format and stack the data, then use first approach to calculate LCC from the stacked dataset.



Working with nested data using purrr

Useful functions:

tidyr::nest(df, cols): creates data frame with cols nested within grouped defined by the non-nesting columns.

tidyr:: unnest(df, cols): unnests a nested column col of a nested data frame.

purrr::map applies a function to each element of a list or vector (ie. each data frame of a nested data frame)

Working with nested data frames

Original data frame

```
iris
A tibble: 150 x 5
   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
          <dbl>
                       <dbl>
                                    <dbl>
                                                 <dbl> <fct>
            5.1
                         3.5
                                                   0.2 setosa
1
                                      1.4
2
            4.9
                         3
                                      1.4
                                                   0.2 setosa
 3
            4.7
                         3.2
                                      1.3
                                                   0.2 setosa
 4
            4.6
                         3.1
                                      1.5
                                                   0.2 setosa
 5
                         3.6
                                      1.4
                                                   0.2 setosa
 6
            5.4
                         3.9
                                      1.7
                                                   0.4 setosa
7
            4.6
                         3.4
                                                   0.3 setosa
8
                         3.4
                                      1.5
                                                   0.2 setosa
9
            4.4
                         2.9
                                      1.4
                                                   0.2 setosa
10
            4.9
                                                   0.1 setosa
                         3.1
                                      1.5
```

Nested data frame

List-column named "data"

Use map to apply function summary to each nested table

```
n iris$data %>% map(summary)
[[1]]
  Sepal.Length
                  Sepal.Width
                                  Petal.Length
                                                  Petal.Width
Min.
        :4.300
                 Min.
                        :2.300
                                 Min.
                                        :1.000
                                                 Min.
                                                         :0.100
1st Ou.:4.800
                 1st Ou.:3.200
                                 1st Ou.:1.400
                                                  1st Ou.:0.200
Median :5.000
                 Median :3.400
                                 Median :1.500
                                                 Median :0.200
        :5.006
                        :3.428
                                                        :0.246
Mean
                 Mean
                                 Mean
                                        :1.462
                                                 Mean
 3rd Ou.:5.200
                 3rd Ou.:3.675
                                 3rd Ou.:1.575
                                                  3rd Ou.:0.300
        :5.800
Max.
                 Max.
                        :4.400
                                 Max.
                                        :1.900
                                                 Max.
                                                         :0.600
[[2]]
 Sepal.Length
                 Sepal.Width
                                 Petal.Length
                                                Petal.Width
Min.
        :4.900
                 Min.
                        :2.000
                                 Min.
                                        :3.00
                                                Min.
                                                        :1.000
```

Working with nested data frames

Apply base R function **summary** to each nested table and add results to original nested df

```
n_iris %>% mutate(summary = map(data, summary))
A tibble: 3 x 3
Species data summary
<fct> tist> <list>
1 setosa <tibble [50 x 4]> 
2 versicolor <tibble [50 x 4]> 
3 virginica <tibble [50 x 4]>
```

Use formula version to supply arguments to function (in this case 1m)

Use ".x" to pass the df in the first argument to map to the mapped function

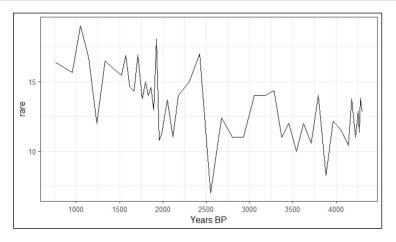
Part 4: Code to aggregate multiple sites using Tidyverse

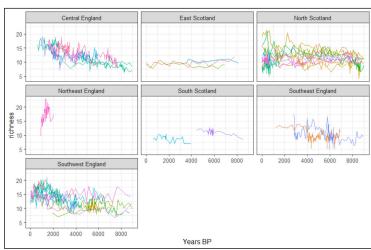
Part 5: Modelling with the Tidyverse

 Calculate palynological richness using rarefaction

Apply model to all sites

Very simple questions:
Which sites show significant trend in richness?
How does richness vary with landscape "openness"





broom for tidying model output

The problem

Tidy(ish) data Model Mot tidy!
No common format

The broom solution

Model -

Convert to tidy with consistent output format for multiple model types (currently >130 included, easy to add your own).

tidy: tibble that summarises model findings (e.g.

coefficients, p-values)

glance: concise one-row summary (e.g. r-squared, degf)

augment: columns original data was modelled on (e.g.

predictions, residuals)

Afternoon (13:30-15:30): Bring your own data

