



Certara R School

Lesson 2: R Basics for Pharmacometrics

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Certara R School

Lesson 3: Exploratory Data Analysis (EDA) Using ggquickedata

6/29/2022 @10am EST

[Register for Lesson 3](#)



What will you learn?

Today we focus on data import and manipulation

- PK Data Overview
 - Creating an R project for your work and Importing files
 - RsNLME Dataset Structure
- Create a RsNLME dataset from CDISC SDTM
 - DM – Demographics
 - EX – Exposure
 - PC – PK Concentrations
 - VS – Vital Signs
- Useful R package `dplyr` functions for data wrangling
- Descriptive statistics
 - Mean concentration by time
 - Demography summary
- Exploratory graphics with `ggplot2`
 - Concentration-time by subject
 - Mean concentration-time by dose group



We will be assembling a script and demonstrating some best practices for this work

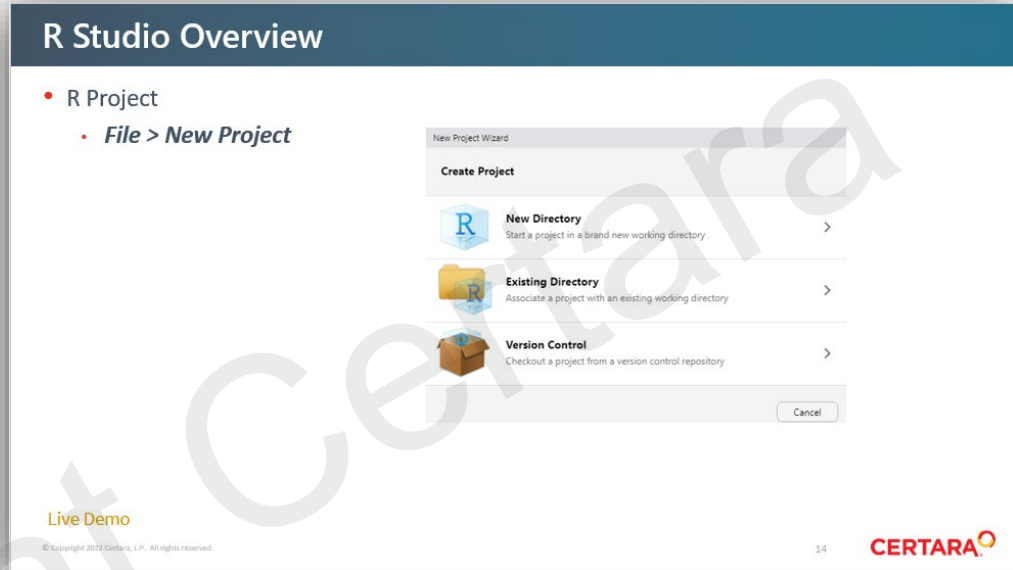
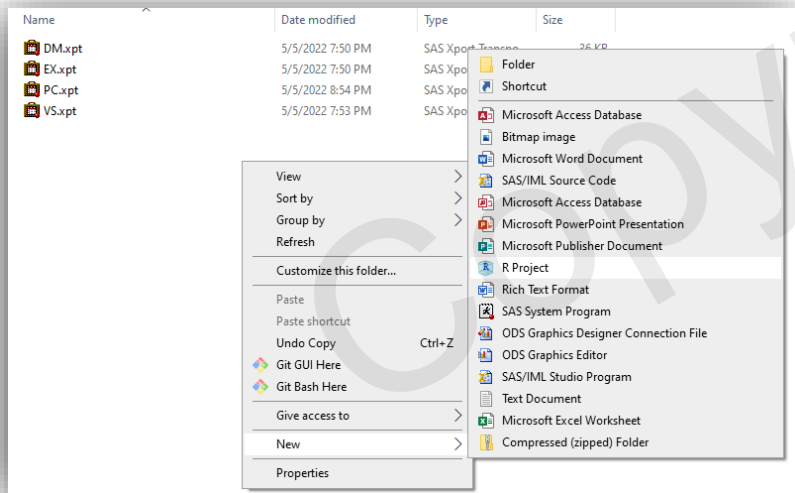
Recap From Last Lecture

Creating an R project for your work

- Last week we covered how to create a new project with RStudio GUI

Pro Tip!

- Create a project with right click in Windows



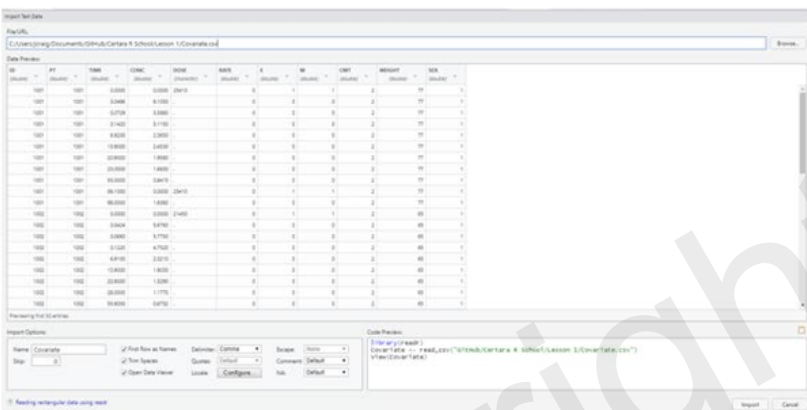
<https://www.anthonyschmidt.co/post/2021-11-19-creating-a-new-r-project-from-the-windows-context-menu/>

Recap from Last Lecture

Importing Files

R Studio Overview

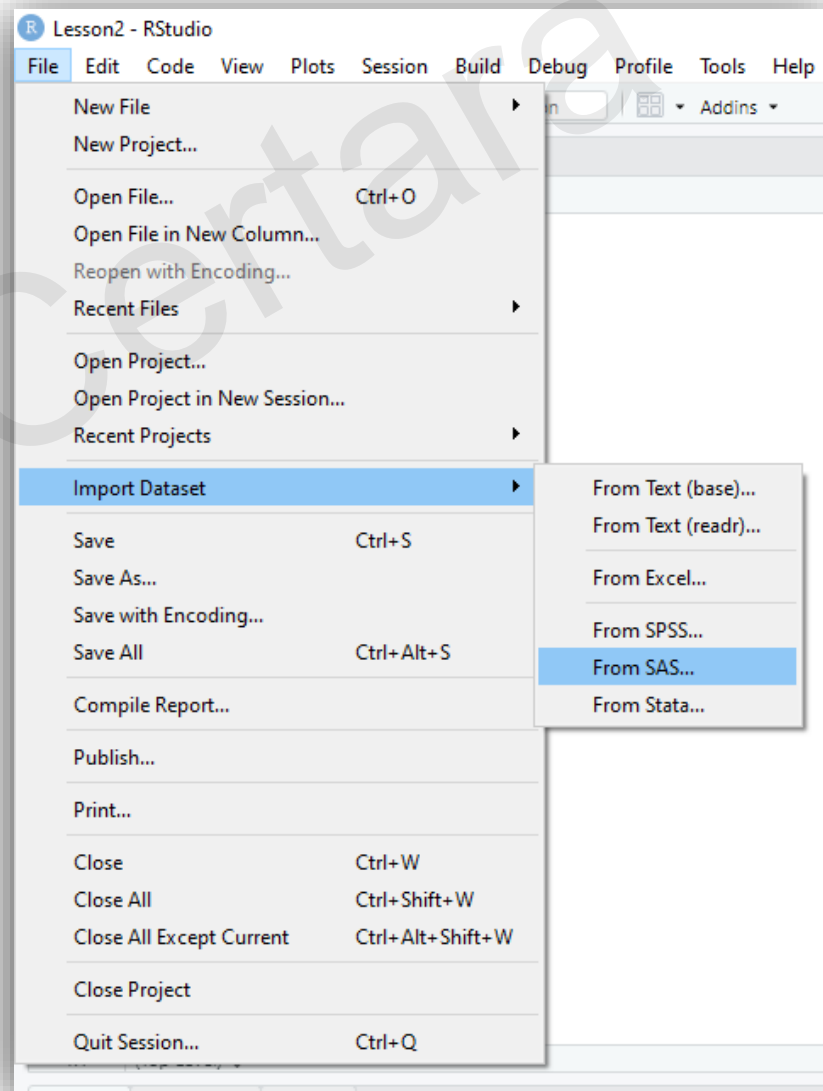
- Importing Data
 - **File > Import Dataset**
 - Import xls
 - Define NA
 - Import CSV
 - Define col types
 - Copy code, update NA argument
 - Importing data with whitespace delimiter



Live Demo

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STDM Source Files

DM: Demography Information

STUDYID	DOMAIN	USUBJID	SUBJID	RFSTDTCT	RFENDTCT	RFXSTDTCT	RFXENDTCT	RFICDTCT	RFPENDTCT	DTHDTCT	DTHFL	SITEID	AGE	AGEU	SEX	RACE	ETHNIC	ARMCD	ARM
SMPSTDYPK	DM	SMPSTDYPK-000001	1	2021-03-02		2021-03-02	2021-06-13	2021-03-01	2021-07-04			123456	56	YEARS	M	WHITE	HISPANIC OR LATINO	A	Treatment Regimen A
SMPSTDYPK	DM	SMPSTDYPK-000002	2	2021-03-02		2021-03-02	2021-06-13	2021-03-01	2021-07-04			123456	45		M	WHITE	NOT HISPANIC OR LATINO	A	Treatment Regimen A
SMPSTDYPK	DM	SMPSTDYPK-000003	3	2021-03-02		2021-03-02	2021-06-13	2021-03-01	2021-07-04			123456	51		M	NATIVE HAWAIIAN OR OTHER PACIFIC ISLANDER	NOT HISPANIC OR LATINO	A	Treatment Regimen A
SMPSTDYPK	DM	SMPSTDYPK-000004	4	2021-03-02		2021-03-02	2021-06-13	2021-03-01	2021-07-04			123456	47		F	WHITE	NOT HISPANIC OR LATINO	A	Treatment Regimen A

EX: Dosing Information

STUDYID	DOMAIN	USUBJID	EXSEQ	EXTRT	EXDOSE	EXDOSU	EXDOSFRM	EXDOSFRQ	EXROUTE	VISITNUM	VISIT	EPOCH	EXSTDTC	EXENDTCT	EXSTDY	EXENDY
SMPSTDYPK	EX	SMPSTDYPK-000001	1	Drug A	5000	mg	TABLET	SINGLE DOSE	ORAL	20	WEEK 1	TREATMENT	2021-03-02T08:00	2021-03-02T08:00	1	1
SMPSTDYPK	EX	SMPSTDYPK-000002	1	Drug A	5000	mg	TABLET	SINGLE DOSE	ORAL	20	WEEK 1	TREATMENT	2021-03-02T08:00	2021-03-02T08:00	1	1
SMPSTDYPK	EX	SMPSTDYPK-000003	1	Drug A	5000	mg	TABLET	SINGLE DOSE	ORAL	20	WEEK 1	TREATMENT	2021-03-02T08:00	2021-03-02T08:00	1	1
SMPSTDYPK	EX	SMPSTDYPK-000004	1	Drug A	5000	mg	TABLET	SINGLE DOSE	ORAL	20	WEEK 1	TREATMENT	2021-03-02T08:00	2021-03-02T08:00	1	1
SMPSTDYPK	EX	SMPSTDYPK-000005	1	Drug A	5000	mg	TABLET	SINGLE DOSE	ORAL	20	WEEK 1	TREATMENT	2021-03-02T08:00	2021-03-02T08:00	1	1

PC: PK (PD) Sampling Information

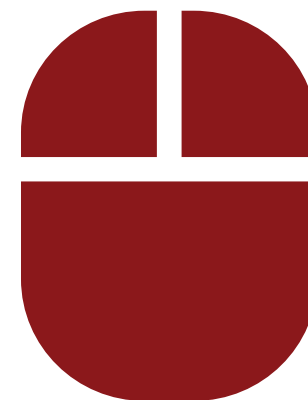
STUDYID	DOMAIN	USUBJID	PCSEQ	PCREFID	PCTESTCD	PCTEST	PCORRES	PCORRESU	PCSTRESC	PCSTRESN	PCSTRESU	PCSTAT	PCREASND	PCNAM	PCSPEC	PCLOQ	VISITNUM	VISIT
SMPSTDYPK	PC	SMPSTDYPK-00...	1	S001345670	AN001	ANALYTE DRU...	BLQ	ug/mL	BLQ		ug/mL			BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	2	S001345671	AN001	ANALYTE DRU...	8.61	ug/mL	8.61	8.61	ug/mL			BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	3	S001345672	AN001	ANALYTE DRU...	19.4	ug/mL	19.4	19.4	ug/mL			BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	4	S001345673	AN001	ANALYTE DRU...	34	ug/mL	34		34	ug/mL		BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	5	S001345674	AN001	ANALYTE DRU...	30.2	ug/mL	30.2	30.2	ug/mL			BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	6	S001345675	AN001	ANALYTE DRU...	31.3	ug/mL	31.3		31.3	ug/mL		BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	7	S001345676	AN001	ANALYTE DRU...	25	ug/mL	25		25	ug/mL		BLUE BELL LABS	PLASMA	0.1	20	WEEK 1
SMPSTDYPK	PC	SMPSTDYPK-00...	8	S001345677	AN001	ANALYTE DRU...	23.4	ug/mL	23.4		23.4	ug/mL		BLUE BELL LABS	PLASMA	0.1	20	WEEK 1

VS: Vital Sign Information

STUDYID	DOMAIN	USUBJID	VSSEQ	VSTESTCD	VSTEST	VSPOS	VSORRES	VSORRESU	VSSTRESC	VSSTRESN	VSSTRESU	VSSTAT	VSREASND	VSBFL	VSDRVFL	VISITNUM	VISIT	EPOCH	VSDTC	VSDY
SMPSTDYPK	VS	SMPSTDYPK-000001	1	WEIGHT	Weight		95	kg	95	95	kg			Y		10	SCREENING	SCREENING	2021-03-01	-1
SMPSTDYPK	VS	SMPSTDYPK-000001	2	WEIGHT	Weight		94	kg	94	94	kg					20	WEEK 1	TREATMENT	2021-03-02	1
SMPSTDYPK	VS	SMPSTDYPK-000002	1	WEIGHT	Weight		65	kg	65	65	kg			Y		10	SCREENING	SCREENING	2021-03-01	-1
SMPSTDYPK	VS	SMPSTDYPK-000002	2	WEIGHT	Weight		64	kg	64	64	kg					20	WEEK 1	TREATMENT	2021-03-02	1
SMPSTDYPK	VS	SMPSTDYPK-000003	1	WEIGHT	Weight		69	kg	69	69	kg			Y		10	SCREENING	SCREENING	2021-03-01	-1
SMPSTDYPK	VS	SMPSTDYPK-000003	2	WEIGHT	Weight		68	kg	68	68	kg					20	WEEK 1	TREATMENT	2021-03-02	1
SMPSTDYPK	VS	SMPSTDYPK-000004	1	WEIGHT	Weight		60	kg	60	60	kg			Y		10	SCREENING	SCREENING	2021-03-01	-1
SMPSTDYPK	VS	SMPSTDYPK-000004	2	WEIGHT	Weight		62	kg	62	62	kg					20	WEEK 1	TREATMENT	2021-03-02	1
SMPSTDYPK	VS	SMPSTDYPK-000005	1	WEIGHT	Weight		72	kg	72	72	kg			Y		10	SCREENING	SCREENING	2021-03-01	-1

Demo – R Script Section 1: Import Data

```
# Section 1: Import Data ----
```



A Note on R Data Objects

Some fundamentals to be aware of

- A **vector** is the most basic data object in R
 - There are six “types”, but for now we look at three
 - A vector can only contain one data type
 - Concept known as “atomic” vector
- A **matrix** is collection of equal length vectors arranged in a two-dimensional rectangular layout
 - A matrix can only contain one data type

double

```
> x<-c(1.1, 3.5, 2.7)
> x
[1] 1.1 3.5 2.7
> typeof(x)
[1] "double"
```

character

```
> x<-c("tree", "dog")
> x
[1] "tree" "dog"
> typeof(x)
[1] "character"
```

logical

```
> x<-c(T,F)
> x
[1] TRUE FALSE
> typeof(x)
[1] "logical"
```

A mixed vector will “coerce” to character

```
> x<-c(1.1, 3.5, 2.7, "dog", "cat", T, F)
> x
[1] "1.1" "3.5" "2.7" "dog" "cat" "TRUE" "FALSE"
> typeof(x)
[1] "character"
```

matrix

```
> x<-c(1.1, 3.5, 2.7)
> y<-c(4, 5.6, 6)
> z<-cbind(x,y)
> z
      x y
[1,] 1.1 4.0
[2,] 3.5 5.6
[3,] 2.7 6.0
> typeof(z)
[1] "double"
> class(z)
[1] "matrix" "array"
```

only one data type allowed

```
> x<-c(1.1, 3.5, 2.7)
> y<-c("tree", "dog", "cat")
> z<-cbind(x,y)
> z
      x y
[1,] "1.1" "tree"
[2,] "3.5" "dog"
[3,] "2.7" "cat"
> typeof(z)
[1] "character"
> class(z)
[1] "matrix" "array"
```


A Note on R Data Objects (cont.)

Some fundamentals to be aware of

- A **data frame** is collection of equal length vectors arranged in a two-dimensional rectangular layout.
 - (a matrix) but....
 - A data frame can contain multiple data types
 - Most commonly used data object for PMX type data
- A **tibble** is a data frame
 - Tweaked to optimize performance in the tidyverse
 - Fewer “default” actions
 - Never converts strings to factors or changes the names of variables
 - More flexibility
 - Can use non-compliant column names (numbers, spaces in names)
 - ...but need to reference these “non-syntactic” names with backticks ``
 - Printing
 - Will only display first 10 rows of large data objects
 - Displays column type
 - Color and font style enhanced display

data frame

```
> x<-c(1.1, 3.5, 2.7)
> y<-c("tree", "dog", "cat")
> z<-data.frame(x,y)
> z
  x     y
1 1.1 tree
2 3.5  dog
3 2.7  cat
> typeof(z)
[1] "list"
> class(z)
[1] "data.frame"
```

A “list” is an R object that contains elements of different types

tibble

```
> x<-c(1.1, 3.5, 2.7)
> y<-c("tree", "dog", "cat")
> z<-tibble(x,y)
> z
# A tibble: 3 x 2
   x     y
<dbl> <chr>
1  1.1 tree
2  3.5  dog
3  2.7  cat
> typeof(z)
[1] "list"
> class(z)
[1] "tbl_df"      "tbl"        "data.frame"
```

Let's Create a RsNLME Dataset!

Study Description

Basic Design and Source Data

- 150 Subjects
- 3 Treatment Groups
 - Single 5, 10, or 20 mg oral dose administered at time=0
- Serial blood samples for PK collected up to 24 hours post-dose
- Desired covariate information in dataset:
 - Age, Weight, Gender, Race, Dose Group
- Source data are SDTM “Standard Data Tabulation Model” datasets

ID	Time	Amt	Conc	Age	Weight	Gender	Race	DoseGrp
1	0	5000	0	56	94	Male	WHITE	5000
1	0.25	0	8.612809	56	94	Male	WHITE	5000
1	0.5	0	19.43682	56	94	Male	WHITE	5000
1	1	0	34.0067	56	94	Male	WHITE	5000
1	2	0	30.2288	56	94	Male	WHITE	5000
1	3	0	31.29961	56	94	Male	WHITE	5000
1	4	0	24.97912	56	94	Male	WHITE	5000
1	6	0	23.37618	56	94	Male	WHITE	5000
1	8	0	23.51309	56	94	Male	WHITE	5000
1	12	0	14.67865	56	94	Male	WHITE	5000
1	16	0	9.073463	56	94	Male	WHITE	5000
1	24	0	5.2962	56	94	Male	WHITE	5000
2	0	5000	0	45	64	Male	WHITE	5000
2	0.25	0	30.40228	45	64	Male	WHITE	5000
2	0.5	0	47.62615	45	64	Male	WHITE	5000
2	1	0	64.42828	45	64	Male	WHITE	5000
2	2	0	100.1783	45	64	Male	WHITE	5000
2	3	0	92.56154	45	64	Male	WHITE	5000
2	4	0	65.26794	45	64	Male	WHITE	5000
2	6	0	49.26316	45	64	Male	WHITE	5000
2	8	0	60.28592	45	64	Male	WHITE	5000
2	12	0	44.24852	45	64	Male	WHITE	5000
2	16	0	41.85031	45	64	Male	WHITE	5000
2	24	0	32.89788	45	64	Male	WHITE	5000

RsNLME Dataset Format Overview

Event by Event History of Dosing, Observations, and Covariate Values

- Each row of the dataset is an “event”
 - Dosing Events
 - Observation Events
 - Other events (covariate value change, etc.)
- Required Columns
 - PK Model
 - A1 or Aa (amount administered central or extravascular)
 - Time
 - CObs (observed concentration)
 - Emax or Linear Model
 - C (independent variable)
 - Eobs (observed effect)
- Many optional columns
 - Steady state, additional, dose interval, rate, duration, mdv, blq, etc.
 - Advanced options covered in a future lecture

ID	Time	Amt	Conc	Age	Weight	Gender	Race	DoseGrp
1	0	5000	0	56	94	Male	WHITE	5000
1	0.25	0	8.612809	56	94	Male	WHITE	5000
1	0.5	0	19.43682	56	94	Male	WHITE	5000
1	1	0	34.0067	56	94	Male	WHITE	5000
1	2	0	30.2288	56	94	Male	WHITE	5000
1	3	0	31.29961	56	94	Male	WHITE	5000
1	4	0	24.97912	56	94	Male	WHITE	5000
1	6	0	23.37618	56	94	Male	WHITE	5000
1	8	0	23.51309	56	94	Male	WHITE	5000
1	12	0	14.67865	56	94	Male	WHITE	5000
1	16	0	9.073463	56	94	Male	WHITE	5000
1	24	0	5.2962	56	94	Male	WHITE	5000
2	0	5000	0	45	64	Male	WHITE	5000
2	0.25	0	30.40228	45	64	Male	WHITE	5000
2	0.5	0	47.62615	45	64	Male	WHITE	5000
2	1	0	64.42828	45	64	Male	WHITE	5000
2	2	0	100.1783	45	64	Male	WHITE	5000
2	3	0	92.56154	45	64	Male	WHITE	5000
2	4	0	65.26794	45	64	Male	WHITE	5000
2	6	0	49.26316	45	64	Male	WHITE	5000
2	8	0	60.28592	45	64	Male	WHITE	5000
2	12	0	44.24852	45	64	Male	WHITE	5000
2	16	0	41.85031	45	64	Male	WHITE	5000
2	24	0	32.89788	45	64	Male	WHITE	5000

RsNLME is flexible on requirements for input data

- Can use any column names you like (except reserved)
- Can use date-times as time variables
 - No need to derive numeric times
- Can use characters for variable values (e.g., M/F)
- Up to 5 ID variables
 - Analysis across multiple studies with repeating ID's?
 - No problem, use Study and ID as ID variables
- Dose information need not be integrated into same dataset as observations
- Covariate values can be missing in dataset
 - Can “fill in” missing covariate data
 - Carry forward
 - Carry backwards
 - Interpolate
- RsNLME does not require time to be sorted
 - Will sort automatically within ID

Caveats

- “Good data housekeeping” is critical to quality analyses
 - Flexible data requirements can allow you to work in a messy house
 - Errors harder to see, unexpected results

- Suggested practice for new modelers
 - Use derived actual times in your dataset
 - 1st event (usually a dose) is time=0, all subsequent events relative to this
 - Avoid long strings for character variables if present
 - No spaces, abbreviate
 - Mind your units!
 - e.g., dose in ug, conc in ug/mL, time in hr will give parameter units in mL and hr
- CL=mL/hr, V=hr

Common Data Manipulation Commands in dplyr

```
> df
```

	ID	Treatment	Dose
1	1	TRT A	5
2	2	Placebo	NA
3	3	TRT B	10
4	4	TRT C	20
5	5	Placebo	NA

arrange:

```
> df %>% arrange(Dose)
```

	ID	Treatment	Dose
1	1	TRT A	5
2	3	TRT B	10
3	4	TRT C	20
4	2	Placebo	NA
5	5	Placebo	NA

```
> df %>% arrange(desc(Dose))
```

	ID	Treatment	Dose
1	4	TRT C	20
2	3	TRT B	10
3	1	TRT A	5
4	2	Placebo	NA
5	5	Placebo	NA

rename:

```
> df %>% rename("AMT" = Dose)
```

	ID	Treatment	AMT
1	1	TRT A	5
2	2	Placebo	NA
3	3	TRT B	10
4	4	TRT C	20
5	5	Placebo	NA

select:

```
> df %>% select(ID,Dose)
```

	ID	Dose
1	1	5
2	2	NA
3	3	10
4	4	20
5	5	NA

filter:

```
> df %>% filter(Treatment != "Placebo")
```

	ID	Treatment	Dose
1	1	TRT A	5
2	3	TRT B	10
3	4	TRT C	20

mutate:

```
> df %>% mutate(DoseMCG = Dose*1000)
```

	ID	Treatment	Dose	DoseMCG
1	1	TRT A	5	5000
2	2	Placebo	NA	NA
3	3	TRT B	10	10000
4	4	TRT C	20	20000
5	5	Placebo	NA	NA

if_else:

```
> df %>% mutate(DoseMCG = if_else(Treatment!="Placebo",Dose*1000, 0))
```

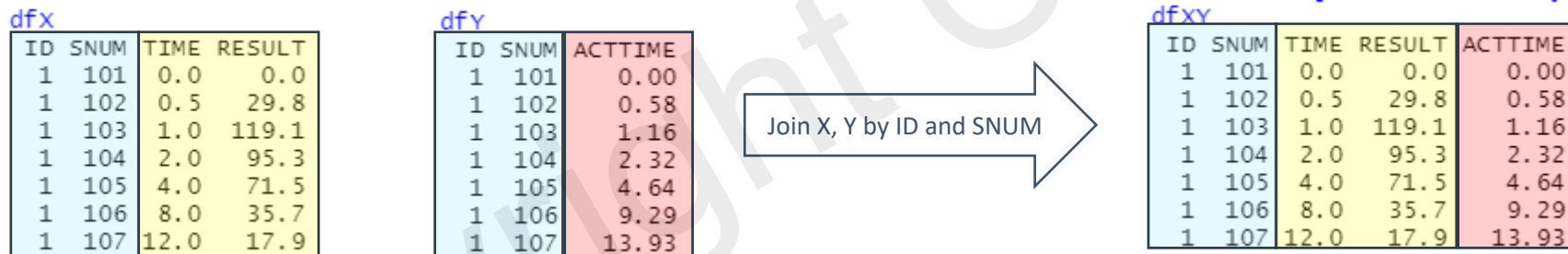
	ID	Treatment	Dose	DoseMCG
1	1	TRT A	5	5000
2	2	Placebo	NA	0
3	3	TRT B	10	10000
4	4	TRT C	20	20000
5	5	Placebo	NA	0

Combining Data From Different Objects

To merge dataframes, use a “join”

- What is a “join”?
- Have 2 dataframes, x and y
- A join command says I want to add (merge) columns from dataframe y to dataframe x, matching on some key

- Example:



ID	SNUM	TIME	RESULT
1	101	0.0	0.0
1	102	0.5	29.8
1	103	1.0	119.1
1	104	2.0	95.3
1	105	4.0	71.5
1	106	8.0	35.7
1	107	12.0	17.9

ID	SNUM	ACTTIME
1	101	0.00
1	102	0.58
1	103	1.16
1	104	2.32
1	105	4.64
1	106	9.29
1	107	13.93

Join X, Y by ID and SNUM

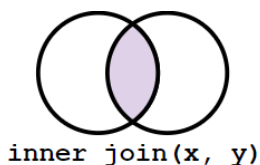
ID	SNUM	TIME	RESULT	ACTTIME
1	101	0.0	0.0	0.00
1	102	0.5	29.8	0.58
1	103	1.0	119.1	1.16
1	104	2.0	95.3	2.32
1	105	4.0	71.5	4.64
1	106	8.0	35.7	9.29
1	107	12.0	17.9	13.93

Joins add columns from y to x, matching rows based on the keys:

- `inner_join()`: includes all rows in x and y
- `left_join()`: includes all rows in x
- `right_join()`: includes all rows in y
- `full_join()`: includes all rows in x or y

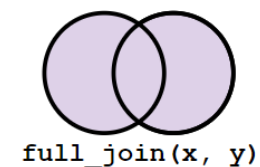
Joins add columns from Y to X, matching rows based on keys

General `dplyr` merging syntax: `join(X, Y, by=key(s))`



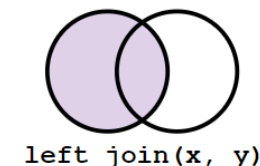
`inner_join(x, y)`

- `inner_join`
 - Only keep rows where key exists in both X and Y



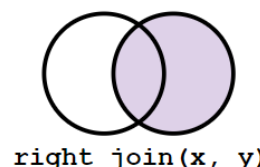
`full_join(x, y)`

- `full_join`
 - Keeps all rows from X and Y



`left_join(x, y)`

- `left_join`
 - Keeps all rows from X
 - Most commonly used join



`right_join(x, y)`

- `right_join`
 - Keeps all rows from Y

X

```
> df1
  ID Treatment
1  1   TRT A
2  2  Placebo
3  3   TRT B
4  4   TRT C
5  5  Placebo
```

Y

```
df2
  ID Dose
1  1    5
3  3   10
4  4   20
6  6   40
```

Add from Y to X

```
inner_join(df1,df2,by="ID")
  ID Treatment Dose
1  1   TRT A    5
3  3   TRT B   10
4  4   TRT C   20
```

```
> df1
  ID Treatment
1  1   TRT A
2  2  Placebo
3  3   TRT B
4  4   TRT C
5  5  Placebo
```

```
df2
  ID Dose
1  1    5
3  3   10
4  4   20
6  6   40
```

```
full_join(df1,df2,by="ID")
  ID Treatment Dose
1  1   TRT A    5
2  2  Placebo  NA
3  3   TRT B   10
4  4   TRT C   20
5  5  Placebo  NA
6  6   <NA>   40
```

```
> df1
  ID Treatment
1  1   TRT A
2  2  Placebo
3  3   TRT B
4  4   TRT C
5  5  Placebo
```

```
df2
  ID Dose
1  1    5
3  3   10
4  4   20
6  6   40
```

```
left_join(df1,df2,by="ID")
  ID Treatment Dose
1  1   TRT A    5
2  2  Placebo  NA
3  3   TRT B   10
4  4   TRT C   20
5  5  Placebo  NA
```

```
> df1
  ID Treatment
1  1   TRT A
2  2  Placebo
3  3   TRT B
4  4   TRT C
5  5  Placebo
```

```
df2
  ID Dose
1  1    5
3  3   10
4  4   20
6  6   40
```

```
right_join(df1,df2,by="ID")
  ID Treatment Dose
1  1   TRT A    5
3  3   TRT B   10
4  4   TRT C   20
6  6   <NA>   40
```

Reshaping

Pivot wider and pivot longer

- `pivot_longer` makes datasets longer by increasing the number of rows and decreasing the number of columns.

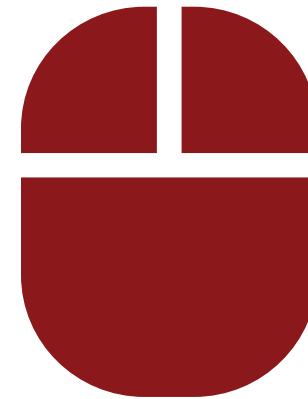
```
> df
# A tibble: 3 x 8
  ID `0` `0.5` `1` `2` `4` `8` `12`
<dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
1     1     0 27.1 108.  86.7  65   32.5  16.3
2     2     0 21.6  86.5  69.2  51.9  25.9   13
3     3     0 22.2  88.9  71.1  53.3  26.7  13.3
> df %>% pivot_longer(!ID, names_to = "TIME", values_to = "RESULT")
# A tibble: 21 x 3
  ID TIME RESULT
<dbl> <chr> <dbl>
1     1 0      0
2     1 0.5    27.1
3     1 1     108.
4     1 2     86.7
5     1 4      65
6     1 8     32.5
7     1 12    16.3
8     2 0      0
9     2 0.5    21.6
10    2 1     86.5
# ... with 11 more rows
```

- `pivot_wider` makes a dataset wider by increasing the number of columns and decreasing the number of rows

```
> dfx
  ID TIME RESULT
1  1 0.0      0.0
2  1 0.5    27.1
3  1 1.0   108.3
4  1 2.0    86.7
5  1 4.0    65.0
6  1 8.0    32.5
7  1 12.0   16.3
8  2 0.0      0.0
9  2 0.5    21.6
10 2 1.0    86.5
11 2 2.0    69.2
12 2 4.0    51.9
13 2 8.0    25.9
14 2 12.0   13.0
15 3 0.0      0.0
16 3 0.5    22.2
17 3 1.0    88.9
18 3 2.0    71.1
19 3 4.0    53.3
20 3 8.0    26.7
21 3 12.0   13.3
> dfx %>% pivot_wider(id_cols = ID, names_from = TIME, values_from = RESULT)
# A tibble: 3 x 8
  ID `0` `0.5` `1` `2` `4` `8` `12`
<dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
1     1     0 27.1 108.  86.7  65   32.5  16.3
2     2     0 21.6  86.5  69.2  51.9  25.9   13
3     3     0 22.2  88.9  71.1  53.3  26.7  13.3
```

Demo – R Script Section 2: Dataset Preparation

```
# Section 2: Dataset Preparation ----
```



Tables in R : gtsummary or flextable?

- `gtsummary` tables offer most comprehensive functionality, combining data summary operations with table output
 - Lacks output support across all core types
 - Only support for one grouping variable
- `flextable` does not perform data summary operations, simply converts `as data.frame` to table output
 - `flextable` does support all core output types however
- More complex data summary operations should be handled with `dplyr`, then convert the resulting `data.frame` to a `flextable` object
- `gtsummary` table objects can also be converted to `flextable`, allowing you to export the table to different output types

Print Engine	Function	HTML	PDF	RTF	Word
gt	<code>as_gt().</code>	😊	⚠️	⚠️	🚫
flextable	<code>as_flex_table().</code>	😊	😊	🚫	😊
huxtable	<code>as_hux_table().</code>	😊	😊	😊	😊
kableExtra	<code>as_kable_extra().</code>	😊	😊	🚫	🚫
kable	<code>as_kable().</code>	😐	😐	😐	😐
tibble	<code>as_tibble().</code>	😞	😞	😞	😞

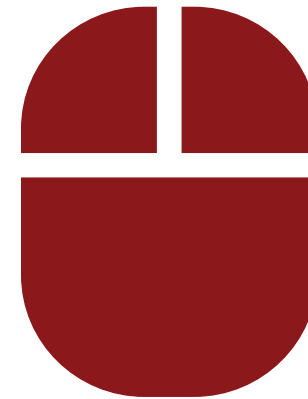


Key

😊	Output fully supported
😐	Formatted output, but missing indentation, footnotes, spanning headers
😞	No formatted output
🚫	Output not supported
⚠️	Under development

Demo – R Script Section 3: Descriptive Statistics Tables

```
# Section 3: Descriptive Statistics Tables ----
```



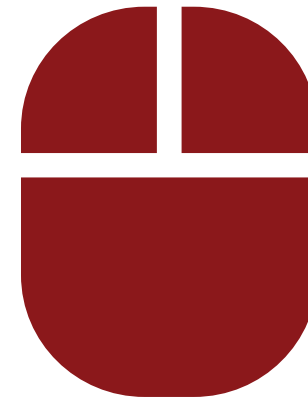
Exploratory Data Analysis with `ggplot2`

- One of the core strengths of R is support for data visualization
- Many plotting packages to choose from:
 - Base R e.g., `plot()`, `hist()`
 - `lattice`
 - `ggplot2`
 - Pharmacometric visualization packages
 - `xpose4`, `xpose`, `Certara.Xpose.NLME`, `ggcertara`
- `ggplot2` offers the most comprehensive plotting functionality in R
- Start with `ggplot()`, supply dataset and aesthetic mappings with `aes()`, then add layers, and optionally split plots (facet) by one or more columns with discrete values.
 - `aes`
 - `x`
 - `y`
 - `color`
 - `group`
 - `layers`
 - `geom_point()`
 - `geom_line()`
 - `geom_bar`

```
</>
ggplot(data, aes(x,y)) +
  geom_point()
```

Demo – R Script Section 4: Exploratory Data Analysis

```
# Section 4: Exploratory Data Analysis ----
```



Questions





Certara R School

Lesson 3: Exploratory Data Analysis (EDA) Using ggquickedata

5/25/2022 @10am EST

[Register for Lesson 3](#)

