My Example Computed Manuscript

Created in Rmarkdown

Jeffrey M. Perkel, Technology Editor, Nature

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A mock computed manuscript created in RStudio using {Rmarkdown}. The {Bookdown} and {Rticles} packages were used to output the text in Springer Nature’s desired manuscript format.

# 1 Introduction

“Literate programming” is a style of programming that uses computational notebooks to weave together code, explanatory text, data and results into a single document, enhancing scientific communication and computational reproducibility.1–3 (These references were added into the document using RStudio’s integration with the open-source Zotero reference manager4 plus the [Better BibTeX](https://retorque.re/zotero-better-bibtex/) Zotero plugin.)

Several platforms for creating such documents exist.5 Typically, these documents interleave code and text ‘blocks’ to build a computational narrative. But some, including [R Markdown](https://rmarkdown.rstudio.com/), [Observable](https://www.observablehq.com), and the [Jupyter Book](https://jupyterbook.org/intro.html) extension to the Jupyter ecosystem, also allow authors to include and execute code “inline” – that is, within the text itself.

This makes it possible to create fully executable manuscripts in which the document itself computes and inserts values and figures into the text rather than requiring authors to input them manually. This is in many ways the ‘killer feature’ of computed manuscripts: it circumvents the possibility that the author will enter an incorrect number, or forget to update a figure or value should new data arise. Among other uses, that allows authors to automatically time-stamp their documents, or insert the current version number of the software they use into their methods. For instance, this document was built at **24 Feb 2022 17:39:06 MST** and calls the following R packages: {tidyverse} ver. **1.3.0**, {ggbeeswarm} ver. **0.6.0** and {bookdown} ver. **0.24**.

In this manuscript, created in RStudio using the R Markdown language, we will demonstrate a more practical example. (An Observable version is [also available](https://observablehq.com/@jperkel/example-executable-observable-notebook).)

# 2 Results

## 2.1 Inline computation

Imagine we are analyzing data from a clinical trial. We have grouped subjects in three bins and measured the concentration of some metabolite. (These data are simulated.)

Rather than analyzing those data and then copying the results into our manuscript, we can use the programming language R to do that in the manuscript itself. Simply enclose the code inside backticks, with the letter r. For instance, we could calculate the circumference and area of a circle:

You could write “A = `r pi \* r^2` and C = `r 2 \* pi \* r`”. Plugging in the radius *r* = **10**, that evaluates to “A = **314.16** and C = **62.83**”.

Returning to our dataset, we can count the rows in our table to determine the number of samples, and insert that into the text. Thus, we have **99** (simulated) subjects in our study (see Table 3.1; see [R/mock\_data.R](https://github.com/jperkel/computed_manuscript/blob/main/R/mock_data.R) in the GitHub repository for code to generate a mock dataset). Note that the tables, figures and sections in this document are numbered automatically thanks to the {bookdown} package.

The average metabolite concentration in this dataset is **185.36** (range: **78 to 298**). We have **32** subjects in Group 1, **43** subjects in Group 2, and **24** in Group 3. (The numbers in **bold face type** throughout this document are computed values.)

## 2.2 Incorporating new data

Now suppose we get another tranche of data (Table 3.2). There are **60** subjects in this new dataset, with an average concentration of **185.13** (range: **77 to 299**).

Combining the two datasets, we have a total of **159** subjects with an average metabolite concentration of **185.28** (range: **77 to 299**). We now have **55** subjects in Group 1, **60** in Group 2, and **44** in Group 3. The concentration distribution for each group in this joint dataset is shown graphically in Figure 2.1.

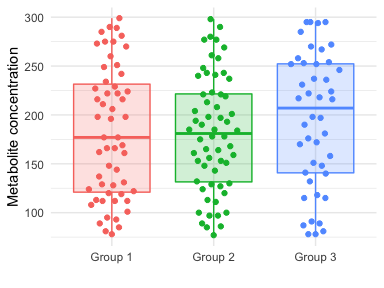


Figure 2.1: Metabolite concentration of clinical trial subjects

## 2.3 Importing a child document

Authors can break long manuscripts into more manageable pieces by placing each chapter or section in their own Markdown file and using the R Markdown child option. Though most of the text (and code) in this document is contained in the file computed\_manuscript.Rmd, the text for this section comes from child\_doc.Rmd. Citations that are created in the child automatically get inserted into the final document, making it possible to create a single, unified bibliography. For instance, here’s a reference for the [R Markdown Cookbook](https://bookdown.org/yihui/rmarkdown-cookbook/).6

In this child document, we’ll add a third set of numbers to our growing dataset (Table 3.3; note that the table, figure and section numbering in this child document matches that of the larger manuscript).

The new dataset describes **50** samples. Folding them into our existing data gives us **209** subjects, with **69** in Group 1, **74** in Group 2, and **66** in Group 3. The new concentration distribution is shown graphically in Figure 2.2.

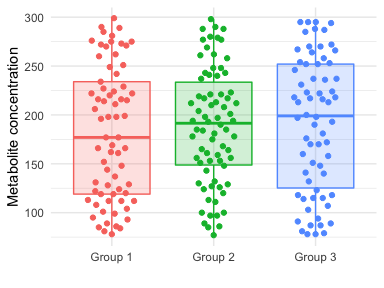


Figure 2.2: Metabolite concentration of final clinical trial dataset

# 3 Code

The following code was used to load, merge, and plot the (simulated) clinical trial data in Figure 2.1:

# load libraries  
library(tidyverse)  
library(ggbeeswarm)  
library(bookdown)

# read in some initial data  
df1 <- read\_csv('data/example-data-1.csv')

# read new dataset  
df2 <- read\_csv('data/example-data-2.csv')

# merge datasets  
final\_data <- rbind(df1, df2)

# create a box-plot with overlaid points  
create\_plot <- function(mytable) {  
 p <- mytable %>%   
 ggplot(aes(x = class, y = conc, fill = class, color = class)) +  
 geom\_boxplot(outlier.shape = NA, alpha = 0.2) +  
 ggbeeswarm::geom\_quasirandom(width = 0.25) +   
 xlab("") +  
 ylab("Metabolite concentration") +   
 theme\_minimal() +  
 theme(legend.position = "none")  
 p  
}

# plot the data  
create\_plot(final\_data)

Table 3.1: Initial subject data

| ID | Class | Conc | | | ID | Class | Conc | | | ID | Class | Conc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID\_1 | Group 2 | 153 | | | ID\_34 | Group 2 | 221 | | | ID\_67 | Group 3 | 148 |
| ID\_2 | Group 1 | 224 | | | ID\_35 | Group 1 | 112 | | | ID\_68 | Group 1 | 281 |
| ID\_3 | Group 2 | 127 | | | ID\_36 | Group 3 | 246 | | | ID\_69 | Group 3 | 295 |
| ID\_4 | Group 2 | 194 | | | ID\_37 | Group 2 | 190 | | | ID\_70 | Group 2 | 111 |
| ID\_5 | Group 1 | 251 | | | ID\_38 | Group 1 | 177 | | | ID\_71 | Group 2 | 132 |
| ID\_6 | Group 1 | 81 | | | ID\_39 | Group 1 | 148 | | | ID\_72 | Group 2 | 261 |
| ID\_7 | Group 2 | 100 | | | ID\_40 | Group 2 | 290 | | | ID\_73 | Group 1 | 122 |
| ID\_8 | Group 1 | 270 | | | ID\_41 | Group 2 | 151 | | | ID\_74 | Group 2 | 124 |
| ID\_9 | Group 2 | 100 | | | ID\_42 | Group 2 | 159 | | | ID\_75 | Group 1 | 234 |
| ID\_10 | Group 1 | 161 | | | ID\_43 | Group 2 | 113 | | | ID\_76 | Group 2 | 184 |
| ID\_11 | Group 3 | 158 | | | ID\_44 | Group 1 | 249 | | | ID\_77 | Group 3 | 272 |
| ID\_12 | Group 3 | 118 | | | ID\_45 | Group 1 | 124 | | | ID\_78 | Group 1 | 242 |
| ID\_13 | Group 2 | 143 | | | ID\_46 | Group 3 | 87 | | | ID\_79 | Group 2 | 277 |
| ID\_14 | Group 2 | 258 | | | ID\_47 | Group 1 | 166 | | | ID\_80 | Group 3 | 236 |
| ID\_15 | Group 3 | 224 | | | ID\_48 | Group 1 | 196 | | | ID\_81 | Group 1 | 101 |
| ID\_16 | Group 3 | 254 | | | ID\_49 | Group 1 | 112 | | | ID\_82 | Group 3 | 218 |
| ID\_17 | Group 3 | 190 | | | ID\_50 | Group 1 | 289 | | | ID\_83 | Group 2 | 130 |
| ID\_18 | Group 2 | 148 | | | ID\_51 | Group 2 | 161 | | | ID\_84 | Group 1 | 128 |
| ID\_19 | Group 1 | 89 | | | ID\_52 | Group 3 | 270 | | | ID\_85 | Group 3 | 252 |
| ID\_20 | Group 2 | 89 | | | ID\_53 | Group 2 | 237 | | | ID\_86 | Group 1 | 198 |
| ID\_21 | Group 3 | 253 | | | ID\_54 | Group 2 | 280 | | | ID\_87 | Group 1 | 169 |
| ID\_22 | Group 3 | 231 | | | ID\_55 | Group 2 | 175 | | | ID\_88 | Group 2 | 185 |
| ID\_23 | Group 1 | 112 | | | ID\_56 | Group 2 | 223 | | | ID\_89 | Group 1 | 216 |
| ID\_24 | Group 2 | 277 | | | ID\_57 | Group 3 | 295 | | | ID\_90 | Group 2 | 185 |
| ID\_25 | Group 2 | 197 | | | ID\_58 | Group 1 | 275 | | | ID\_91 | Group 2 | 97 |
| ID\_26 | Group 2 | 208 | | | ID\_59 | Group 2 | 120 | | | ID\_92 | Group 2 | 165 |
| ID\_27 | Group 2 | 193 | | | ID\_60 | Group 1 | 78 | | | ID\_93 | Group 3 | 89 |
| ID\_28 | Group 3 | 141 | | | ID\_61 | Group 3 | 78 | | | ID\_94 | Group 2 | 221 |
| ID\_29 | Group 1 | 206 | | | ID\_62 | Group 3 | 140 | | | ID\_95 | Group 1 | 162 |
| ID\_30 | Group 2 | 168 | | | ID\_63 | Group 3 | 294 | | | ID\_96 | Group 1 | 131 |
| ID\_31 | Group 2 | 298 | | | ID\_64 | Group 3 | 295 | | | ID\_97 | Group 1 | 93 |
| ID\_32 | Group 1 | 144 | | | ID\_65 | Group 3 | 285 | | | ID\_98 | Group 2 | 240 |
| ID\_33 | Group 2 | 241 | | | ID\_66 | Group 2 | 129 | | | ID\_99 | Group 2 | 86 |

Table 3.2: Second batch of subject data

| ID | Class | Conc | | | ID | Class | Conc | | | ID | Class | Conc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID\_100 | Group 2 | 219 | | | ID\_120 | Group 2 | 85 | | | ID\_140 | Group 2 | 77 |
| ID\_101 | Group 2 | 243 | | | ID\_121 | Group 3 | 181 | | | ID\_141 | Group 1 | 299 |
| ID\_102 | Group 2 | 213 | | | ID\_122 | Group 3 | 216 | | | ID\_142 | Group 3 | 222 |
| ID\_103 | Group 1 | 177 | | | ID\_123 | Group 1 | 222 | | | ID\_143 | Group 1 | 85 |
| ID\_104 | Group 3 | 197 | | | ID\_124 | Group 3 | 252 | | | ID\_144 | Group 1 | 273 |
| ID\_105 | Group 2 | 198 | | | ID\_125 | Group 1 | 166 | | | ID\_145 | Group 3 | 115 |
| ID\_106 | Group 1 | 120 | | | ID\_126 | Group 2 | 204 | | | ID\_146 | Group 1 | 290 |
| ID\_107 | Group 3 | 170 | | | ID\_127 | Group 2 | 243 | | | ID\_147 | Group 2 | 269 |
| ID\_108 | Group 3 | 78 | | | ID\_128 | Group 3 | 198 | | | ID\_148 | Group 2 | 97 |
| ID\_109 | Group 1 | 129 | | | ID\_129 | Group 1 | 119 | | | ID\_149 | Group 1 | 229 |
| ID\_110 | Group 1 | 137 | | | ID\_130 | Group 1 | 198 | | | ID\_150 | Group 3 | 176 |
| ID\_111 | Group 3 | 217 | | | ID\_131 | Group 3 | 151 | | | ID\_151 | Group 2 | 164 |
| ID\_112 | Group 1 | 227 | | | ID\_132 | Group 3 | 115 | | | ID\_152 | Group 3 | 172 |
| ID\_113 | Group 3 | 81 | | | ID\_133 | Group 3 | 237 | | | ID\_153 | Group 1 | 222 |
| ID\_114 | Group 2 | 248 | | | ID\_134 | Group 2 | 178 | | | ID\_154 | Group 1 | 285 |
| ID\_115 | Group 1 | 211 | | | ID\_135 | Group 1 | 275 | | | ID\_155 | Group 2 | 153 |
| ID\_116 | Group 1 | 113 | | | ID\_136 | Group 2 | 178 | | | ID\_156 | Group 3 | 132 |
| ID\_117 | Group 1 | 216 | | | ID\_137 | Group 3 | 267 | | | ID\_157 | Group 2 | 156 |
| ID\_118 | Group 3 | 91 | | | ID\_138 | Group 1 | 95 | | | ID\_158 | Group 1 | 260 |
| ID\_119 | Group 3 | 258 | | | ID\_139 | Group 1 | 108 | | | ID\_159 | Group 2 | 201 |

Table 3.3: Third batch of subject data

| ID | Class | Conc | | | ID | Class | Conc | | | ID | Class | Conc |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ID\_160 | Group 2 | 210 | | | ID\_177 | Group 2 | 288 | | | ID\_194 | Group 3 | 123 |
| ID\_161 | Group 3 | 107 | | | ID\_178 | Group 1 | 262 | | | ID\_195 | Group 2 | 212 |
| ID\_162 | Group 2 | 262 | | | ID\_179 | Group 2 | 217 | | | ID\_196 | Group 1 | 99 |
| ID\_163 | Group 1 | 215 | | | ID\_180 | Group 3 | 87 | | | ID\_197 | Group 3 | 264 |
| ID\_164 | Group 1 | 220 | | | ID\_181 | Group 3 | 266 | | | ID\_198 | Group 2 | 279 |
| ID\_165 | Group 3 | 288 | | | ID\_182 | Group 3 | 79 | | | ID\_199 | Group 2 | 126 |
| ID\_166 | Group 3 | 287 | | | ID\_183 | Group 1 | 152 | | | ID\_200 | Group 1 | 276 |
| ID\_167 | Group 3 | 213 | | | ID\_184 | Group 3 | 223 | | | ID\_201 | Group 3 | 213 |
| ID\_168 | Group 1 | 84 | | | ID\_185 | Group 3 | 118 | | | ID\_202 | Group 2 | 212 |
| ID\_169 | Group 3 | 160 | | | ID\_186 | Group 1 | 214 | | | ID\_203 | Group 1 | 104 |
| ID\_170 | Group 2 | 194 | | | ID\_187 | Group 3 | 200 | | | ID\_204 | Group 1 | 199 |
| ID\_171 | Group 1 | 119 | | | ID\_188 | Group 1 | 271 | | | ID\_205 | Group 1 | 272 |
| ID\_172 | Group 3 | 218 | | | ID\_189 | Group 3 | 237 | | | ID\_206 | Group 1 | 86 |
| ID\_173 | Group 2 | 217 | | | ID\_190 | Group 3 | 170 | | | ID\_207 | Group 2 | 181 |
| ID\_174 | Group 3 | 103 | | | ID\_191 | Group 2 | 156 | | | ID\_208 | Group 3 | 114 |
| ID\_175 | Group 3 | 94 | | | ID\_192 | Group 2 | 288 | | | ID\_209 | Group 2 | 248 |
| ID\_176 | Group 3 | 270 | | | ID\_193 | Group 3 | 193 | | |  |  |  |

# 4 Colophon

This manuscript was built at **24 Feb 2022 17:39:07 MST** using the following computational environment and dependencies:

## R version 4.0.4 (2021-02-15)  
## Platform: x86\_64-apple-darwin17.0 (64-bit)  
## Running under: macOS Big Sur 10.16  
##   
## Matrix products: default  
## BLAS: /Library/Frameworks/R.framework/Versions/4.0/Resources/lib/libRblas.dylib  
## LAPACK: /Library/Frameworks/R.framework/Versions/4.0/Resources/lib/libRlapack.dylib  
##   
## locale:  
## [1] en\_US.UTF-8/en\_US.UTF-8/en\_US.UTF-8/C/en\_US.UTF-8/en\_US.UTF-8  
##   
## attached base packages:  
## [1] stats graphics grDevices utils datasets methods base   
##   
## other attached packages:  
## [1] bookdown\_0.24 ggbeeswarm\_0.6.0 forcats\_0.5.1 stringr\_1.4.0   
## [5] dplyr\_1.0.5 purrr\_0.3.4 readr\_2.1.1 tidyr\_1.1.3   
## [9] tibble\_3.1.6 ggplot2\_3.3.3 tidyverse\_1.3.0   
##   
## loaded via a namespace (and not attached):  
## [1] Rcpp\_1.0.7 lubridate\_1.8.0 assertthat\_0.2.1 digest\_0.6.29   
## [5] utf8\_1.2.2 R6\_2.5.1 cellranger\_1.1.0 backports\_1.2.1   
## [9] reprex\_2.0.1 evaluate\_0.14 highr\_0.9 httr\_1.4.2   
## [13] pillar\_1.6.4 rlang\_0.4.12 readxl\_1.3.1 rstudioapi\_0.13   
## [17] rmarkdown\_2.11 labeling\_0.4.2 bit\_4.0.4 munsell\_0.5.0   
## [21] broom\_0.7.6 compiler\_4.0.4 vipor\_0.4.5 modelr\_0.1.8   
## [25] xfun\_0.29 pkgconfig\_2.0.3 htmltools\_0.5.2 tidyselect\_1.1.1  
## [29] fansi\_1.0.0 crayon\_1.4.2 tzdb\_0.2.0 dbplyr\_2.1.0   
## [33] withr\_2.4.3 grid\_4.0.4 jsonlite\_1.7.2 gtable\_0.3.0   
## [37] lifecycle\_1.0.1 DBI\_1.1.1 magrittr\_2.0.1 scales\_1.1.1   
## [41] cli\_3.1.0 stringi\_1.7.6 vroom\_1.5.7 farver\_2.1.0   
## [45] fs\_1.5.2 xml2\_1.3.3 ellipsis\_0.3.2 generics\_0.1.1   
## [49] vctrs\_0.3.8 tools\_4.0.4 bit64\_4.0.5 glue\_1.6.0   
## [53] beeswarm\_0.4.0 hms\_1.1.1 parallel\_4.0.4 fastmap\_1.1.0   
## [57] yaml\_2.2.1 colorspace\_2.0-0 rvest\_1.0.2 knitr\_1.37   
## [61] haven\_2.3.1

The current Git commit details are:

## [9906399] 2022-02-25: Fix link to Observable example.

# References

1. Shen, H. [Interactive notebooks: Sharing the code](https://doi.org/10.1038/515151a). *Nature* **515**, 151–152 (2014).

2. Perkel, J. M. [A toolkit for data transparency takes shape](https://doi.org/10.1038/d41586-018-05990-5). *Nature* **560**, 513–515 (2018).

3. Perkel, J. M. [Why Jupyter is data scientists’ computational notebook of choice](https://doi.org/10.1038/d41586-018-07196-1). *Nature* **563**, 145–146 (2018).

4. Perkel, J. M. [Streamline your writing and collaborations with these reference managers](https://doi.org/10.1038/d41586-020-02491-2). *Nature* **585**, 149–150 (2020).

5. Perkel, J. M. [Reactive, reproducible, collaborative: computational notebooks evolve](https://doi.org/10.1038/d41586-021-01174-w). *Nature* **593**, 156–157 (2021).

6. Xie, Y., Dervieux, C. & Riederer, E. *R Markdown Cookbook*. (Chapman and Hall/CRC, 2020).