

Design of Experiments

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Chapter 1

About

This material is being developed by Jordi Cuadros (<https://orcid.org/0000-0001-6513-9140>), Laura Fernández Ruano (<https://orcid.org/0000-0001-9879-781X>) and Vanessa Serrano (<https://orcid.org/0000-0001-6572-0680>) as a reference material for a Master's course in Design of Experiments at IQS Universitat Ramon Llull (<http://www.iqs.url.edu>) in Barcelona, Spain. First version (a draft) was published on September 2022.

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1.1 License and contributing

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Should you be interested in contributing to this work, suggest corrections or improvements, or just say thanks, feel free to reach the authors at jordi.cuadros@iqs.url.edu.

Chapter 2

Experimenting

Experimenting is a common task in any scientific endeavor. However, and this is not uncommon, being a common task does not warrant a full comprehension of it.

Let's refresh here some fundamental concepts.

2.1 Why do we experiment? The causality problem**2.2 The elements of an experiment****2.2.1 A basic schema for an experiment****2.2.2 Types of variables****2.2.3 Data types****2.3 Validity of an experiment****2.3.1 Internal validity****2.3.2 External validity****2.4 Running an experiment****2.4.1 Replication and repetition****2.4.2 Randomization****2.5 To explore further****2.5.1 Hierarchy of evidence**

https://en.wikipedia.org/wiki/Hierarchy_of_evidence

Chapter 3

Analyzing an experiment

3.1 Variables, types and levels

3.2 Compiling the experimental matrix

3.3 Analyzing the experiment

3.3.1 Strength

3.3.2 Resolution

3.3.3 Orthogonality

3.3.4 Confounded variables

3.3.5 Optimality

3.3.6 Efficacy

3.3.7 Sphericity

3.4 Identifying relevant contributions

3.4.1 Pareto chart of the effects

3.4.2 Pareto chart of the contributions

3.4.3 Normal plot

3.4.4 Half-normal plot

3.5 Visualizing results, effects and interactions

3.5.1 Main effects plots

3.5.2 Interaction plots

Chapter 4

One factor experiments

4.1 Two-level experiments

4.2 Multiple-level experiments

4.2.1 Quantitative variables

4.2.2 Nominal levels

4.3 To explore further

4.3.1 Single-subject experiments

4.3.2 Salomon design

Chapter 5

Full factorial designs

5.1 OFAT and their limitations

5.2 Full factorial designs

5.2.1 Two-levels factorial designs

5.2.1.1 Standard coding of the experimental conditions

5.2.1.2 Yates order

5.2.2 Multiple-levels factorial designs

5.2.3 Mixed-levels factorial designs

Database: <http://neilsloane.com/oadir/>

5.3 Degrees of freedom**5.4 Interactions and error****5.5 To explore further****5.5.1 Blocking****5.5.2 Latin and grecolatin square**

https://en.wikipedia.org/wiki/Mutually_orthogonal_Latin_squares

5.5.3 Nested, split-plot, split-split and strip-strip designs**5.5.4 BIBD**

Chapter 6

Fractional and saturated factorial designs

6.1 Fractional factorial designs

6.1.1 Two-levels fractional factorial design

6.1.2 Resolution of a design

6.1.3 Alias structure and design generator

6.2 Saturated factorial designs

6.3 Plackett-Burman designs

6.4 Taguchi's approach to orthogonal arrays

6.4.1 Linear graphs and interaction tables

6.5 Follow-up

6.5.1 Follow-up designs

6.5.2 Confirmatory runs

6.6 To explore further

6.6.1 Adding center points

6.6.2 Definitive screening designs

Chapter 7

Non orthogonal arrays

7.1 Modified Taguchi's orthogonal arrays (Special designs)

7.1.1 Column upgrading/merging

7.1.2 Dummy treatment/level or column downgrading/degrading

7.1.3 Idle column

7.1.4 Combination design

7.2 Optimal designs

7.2.1 Optimality criteria

7.3 Supersaturated designs

Chapter 8

Taguchi Robust Design strategy

8.1 Noise and control factors

8.2 Inner and outer arrays designs

8.3 Two-step optimization technique

Chapter 9

Surface response designs

- 9.1 Three-level full factorial designs**
- 9.2 Box-Wilson central composite designs**
- 9.3 Box-Behnken designs**
- 9.4 Doehlert designs**
- 9.5 Sequential design of experiments**
- 9.6 To explore further**
 - 9.6.1 Optimal designs for RSM**

Chapter 10

Sequential optimization

10.1 EVOP

10.2 Simplex

Chapter 11

Advanced and uncovered topics

11.1 Designs for nonlinear effects

11.2 Designs for systems with restrictions

11.2.1 Mixtures designs

11.3 Designs for computer experiments

11.3.1 Space-filling designs

<https://link.springer.com/content/pdf/10.1007/s00362-021-01249-w.pdf>

11.4 Desigsn with random levels

References

- Allaire, J., Xie, Y., McPherson, J., Luraschi, J., Ushey, K., Atkins, A., Wickham, H., Cheng, J., Chang, W., & Iannone, R. (2022). *Rmarkdown: Dynamic documents for r*. <https://CRAN.R-project.org/package=rmarkdown>
- Arnold, J. B. (2021). *Ggthemes: Extra themes, scales and geoms for ggplot2*. <https://github.com/jrnold/ggthemes>
- Box, G. E., Hunter, J. S., & Hunter, W. G. (2005). *Statistics for experimenters: Design, discovery and innovation* (2nd ed., Vol. 639). Wiley-Interscience.
- Darócz, G., & Tsegelskyi, R. (2022). *Pander: An r pandoc writer*. <https://rapporter.github.io/pander/>
- Garnier, S. (2021a). *Viridis: Colorblind-friendly color maps for r*. <https://CRAN.R-project.org/package=viridis>
- Garnier, S. (2021b). *viridisLite: Colorblind-friendly color maps (lite version)*. <https://CRAN.R-project.org/package=viridisLite>
- Grothendieck, G. (2018). *Gsubfn: Utilities for strings and function arguments*. <https://github.com/ggrothendieck/gsubfn>
- Grothendieck, G., Kates, L., & Petzoldt, T. (2016). *Proto: Prototype object-based programming*. <https://github.com/hadley/proto>
- Harding, T., Tusell, F., & Schafer, J. L. (2012). *Cat: Analysis of categorical-variable datasets with missing values*. <http://www.stat.psu.edu/~jls/misoftwa.html#aut>
- Heckert, N., Filliben, J., Croarkin, C., Hembree, B., Guthrie, W., Tobias, P., & Prinz, J. (2002). *Handbook 151: NIST/SEMATECH e-handbook of statistical methods*. NIST Interagency/Internal Report (NISTIR), National Institute of Standards; Technology, Gaithersburg, MD. <https://www.itl.nist.gov/div898/handbook/>
- Henry, L., & Wickham, H. (2020). *Purrr: Functional programming tools*. <https://CRAN.R-project.org/package=purrr>
- Hester, J., Wickham, H., & Bryan, J. (2021). *Vroom: Read and write rectangular text data quickly*. <https://CRAN.R-project.org/package=vroom>
- Minitab, L. (2022). *Minitab 18 support*. <https://support.minitab.com/en-us/minitab/18/>
- Montgomery, D. C. (2019). *Design and analysis of experiments*. John Wiley & Sons.
- Müller, K., & Wickham, H. (2021). *Tibble: Simple data frames*. <https://CRAN>.

- R-project.org/package=tibble
- Myers, R. H., Montgomery, D. C., & Anderson-Cook, C. M. (2016). *Response surface methodology: Process and product optimization using designed experiments*. John Wiley & Sons.
- Park, S. H., & Antony, J. (2008). *Robust design for quality engineering and six sigma*. World Scientific.
- R Core Team. (2022). *R: A language and environment for statistical computing*. R Foundation for Statistical Computing. <https://www.R-project.org/>
- Ren, K., & Russell, K. (2021). *Formattable: Create formattable data structures*. <https://CRAN.R-project.org/package=formattable>
- Temple Lang, D. (2022). *XML: Tools for parsing and generating XML within r and s-plus*. <http://www.omegahat.net/RXML/>
- Tennekes, M. (2021). *Treemap: Treemap visualization*. <https://CRAN.R-project.org/package=treemap>
- The Pennsylvania State University. (2022). *STAT 503 design of experiments*. <https://online.stat.psu.edu/stat503/>
- Warnes, G. R., Bolker, B., Bonebakker, L., Gentleman, R., Huber, W., Liaw, A., Lumley, T., Maechler, M., Magnusson, A., Moeller, S., Schwartz, M., & Venables, B. (2022). *Gplots: Various r programming tools for plotting data*. <https://github.com/talgalili/gplots>
- Wickham, H. (2016). *ggplot2: Elegant graphics for data analysis*. Springer-Verlag New York. <https://ggplot2.tidyverse.org>
- Wickham, H. (2019). *Stringr: Simple, consistent wrappers for common string operations*. <https://CRAN.R-project.org/package=stringr>
- Wickham, H. (2021a). *Forcats: Tools for working with categorical variables (factors)*. <https://CRAN.R-project.org/package=forcats>
- Wickham, H. (2021b). *Tidyverse: Easily install and load the tidyverse*. <https://CRAN.R-project.org/package=tidyverse>
- Wickham, H., Averick, M., Bryan, J., Chang, W., McGowan, L. D., François, R., Grolemund, G., Hayes, A., Henry, L., Hester, J., Kuhn, M., Pedersen, T. L., Miller, E., Bache, S. M., Müller, K., Ooms, J., Robinson, D., Seidel, D. P., Spinu, V., ... Yutani, H. (2019). Welcome to the tidyverse. *Journal of Open Source Software*, 4(43), 1686. <https://doi.org/10.21105/joss.01686>
- Wickham, H., Chang, W., Henry, L., Pedersen, T. L., Takahashi, K., Wilke, C., Woo, K., Yutani, H., & Dunnington, D. (2021). *ggplot2: Create elegant data visualisations using the grammar of graphics*. <https://CRAN.R-project.org/package=ggplot2>
- Wickham, H., François, R., Henry, L., & Müller, K. (2022). *Dplyr: A grammar of data manipulation*. <https://CRAN.R-project.org/package=dplyr>
- Wickham, H., & Girlich, M. (2022). *Tidyr: Tidy messy data*. <https://CRAN.R-project.org/package=tidyr>
- Wickham, H., Hester, J., & Bryan, J. (2022). *Readr: Read rectangular text data*. <https://CRAN.R-project.org/package=readr>
- Wickham, H., & Seidel, D. (2022). *Scales: Scale functions for visualization*. <https://CRAN.R-project.org/package=scales>
- Xie, Y. (2014). Knitr: A comprehensive tool for reproducible research in R.

- In V. Stodden, F. Leisch, & R. D. Peng (Eds.), *Implementing reproducible computational research*. Chapman; Hall/CRC. <http://www.crcpress.com/product/isbn/9781466561595>
- Xie, Y. (2015). *Dynamic documents with R and knitr* (2nd ed.). Chapman; Hall/CRC. <https://yihui.org/knitr/>
- Xie, Y. (2016). *Bookdown: Authoring books and technical documents with R markdown*. Chapman; Hall/CRC. <https://bookdown.org/yihui/bookdown>
- Xie, Y. (2022a). *Bookdown: Authoring books and technical documents with r markdown*. <https://CRAN.R-project.org/package=bookdown>
- Xie, Y. (2022b). *Knitr: A general-purpose package for dynamic report generation in r*. <https://yihui.org/knitr/>
- Xie, Y., Allaire, J. J., & Grolemund, G. (2018). *R markdown: The definitive guide*. Chapman; Hall/CRC. <https://bookdown.org/yihui/rmarkdown>
- Xie, Y., Cheng, J., & Tan, X. (2022). *DT: A wrapper of the JavaScript library DataTables*. <https://github.com/rstudio/DT>
- Xie, Y., Dervieux, C., & Riederer, E. (2020). *R markdown cookbook*. Chapman; Hall/CRC. <https://bookdown.org/yihui/rmarkdown-cookbook>
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