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DESIGN OF EXPERIMENTS & MULTIPLE RESPONSE OPTIMIZATION

FATHER OF DOE

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WHY DESIGN OF EXPERIMENTS?

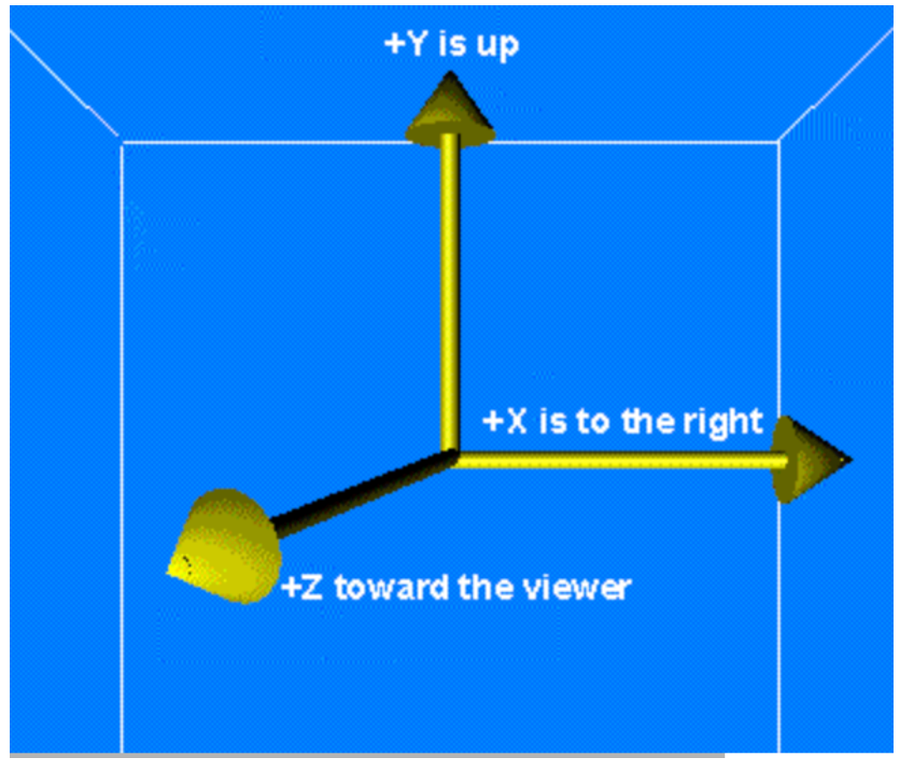
- Design of Experiments [DOE] provides the optimal mathematical solutions to conduct univariate and multivariate prospective (forward-looking) experiments.
- One Factor At a Time [OFAT] experiments, by comparison, show only a portion of inference, compared with DOE plans.
- OFAT models can be misleading, because they do not account for common interaction or polynomial effects.
- But how does DOE work its magic?

DESIGN OF EXPERIMENTS

THE UNDERLYING STRUCTURE

ORTHOGONAL DESIGN

- DOE provides optimal efficiency by creating orthogonal, or near-orthogonal designs.
- DOE systematically changes multiple input settings, simultaneously, and estimates interaction effects.



http://www.euclideanspace.com/maths/algebra/matrix/orthogonal/index.htm

- This leads to better inference regarding phenomenological causality compared with models based on observational data.
- Designs may be modified to incorporate covariates and account for the difficulty in changing the settings of input factors.

ORTHOGONAL DESIGN

- DOE provides optimal efficiency by creating orthogonal, or near-orthogonal designs.
- + stands for ‘on’ or ‘True’ (boolean) or ‘high’ (continuous).

		① Factor Assignment						
		Main Effects ③			Interactions ④			
		A	B	C	D (A-B)	E (A-C)	F (B-C)	G (A-B-C)
② Tests	1	–	–	–	+	+	+	–
	2	+	–	–	–	–	+	+
	3	–	+	–	–	+	–	+
	4	+	+	–	+	–	–	–
	5	–	–	+	+	–	–	+
	6	+	–	+	–	+	–	–
	7	–	+	+	–	–	+	–
	8	+	+	+	+	+	+	+

Design Of Experiments (DOE)

- - is ‘off’, ‘false’, ‘low’. (One should also include mid-points)
- Constraints may be added to ensure DOE stays within budget by limiting the number of runs, and reassessing which designs are optimal based on the number of available runs/tests.

MULTIPLE RESPONSE OPTIMIZATION

A BRIEF INTRODUCTION

MULTIPLE RESPONSE OPTIMIZATION

- Why optimize one outcome, when you can do so for multiple outcomes (responses) at once? **Often, more than one outcome is important…**
- You can do it easily with Multiple Response Optimization [MRO]!
- Uses individual and collective **Desirability Functions [DF]**:
  - Minimum
  - Maximum

$$d_r^{min} = \begin{cases} 0 & \text{if } f_r(\mathbf{x}) > B \\ \left(\frac{f_r(\mathbf{x})-B}{A-B}\right)^s & \text{if } A \leq f_r(\mathbf{x}) \leq B \\ 1 & \text{if } f_r(\mathbf{x}) < A \end{cases} \qquad d_r^{max} = \begin{cases} 0 & \text{if } f_r(\mathbf{x}) < A \\ \left(\frac{f_r(\mathbf{x})-A}{B-A}\right)^s & \text{if } A \leq f_r(\mathbf{x}) \leq B \\ 1 & \text{if } f_r(\mathbf{x}) > B \end{cases}$$

- Target (when most desirable outcome falls between Min and Max)
- Composite (Optimizes all DFs, together, to inform a final decision)
- The Full Details: https://cran.r-project.org/web/packages/desirability/vignettes/desirability.pdf

DESIGN OF EXPERIMENTS

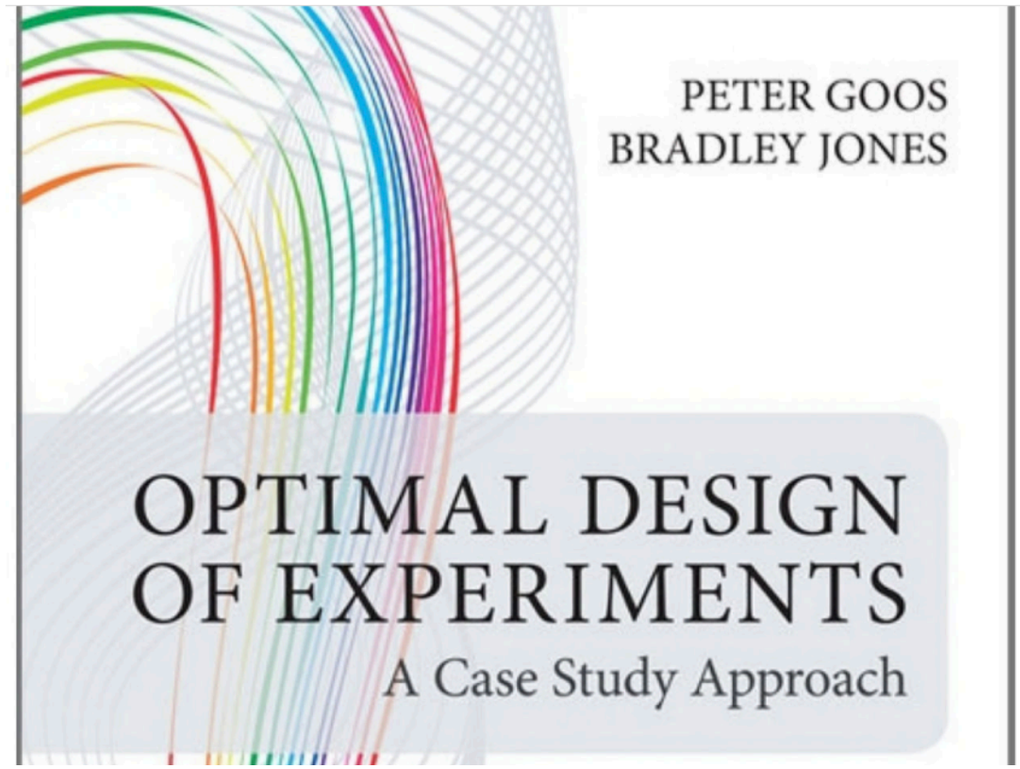
READING & RESOURCES

RESOURCES

- pyDOE - https://pypi.org/project/pyDOE/
  https://pythonhosted.org/pyDOE/
- It seems that Data Science continues to learn from its older sibling, statistics…
- Data Camp just launched a new course in R to teach DOE
  https://www.datacamp.com/courses/experimental-design-in-r
- Check out Bradley Jones and his optimal designs, using JMP Discovery Software, by SAS. www.jmp.com
- R package:
  https://cran.r-project.org/web/packages/desirability/index.html

RECOMMENDED READING

- Optimal Design of Experiments: A Case Study Approach
  Peter Goos, Bradley Jones; SAS



- Also…
- For a general survey, the JMP community is great. You can access free materials on DOE, here:
- https://www.jmp.com/en_us/applications/design-of-experiments.html
- http://j.mp/2Huob8f

THANK YOU

FOR

LISTENING!