WILLIAM BAUM

DESIGN OF EXPERIMENTS & MULTIPLE RESPONSE OPTIMIZATION

FATHER OF DOE

SIR RONALD FISCHER

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.
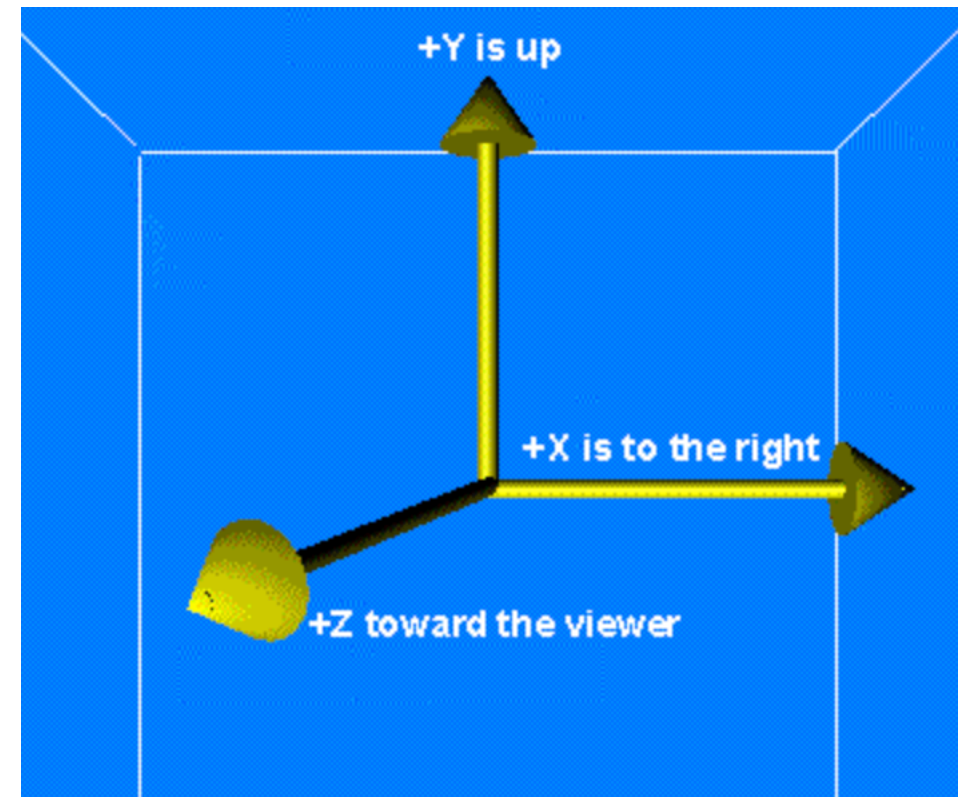
▸ But how does DOE work its magic?

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 thereby 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).

▸ - is 'off', 'false', 'low'.   (One can also include mid-points for continuous variables)

▸ 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.

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)

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

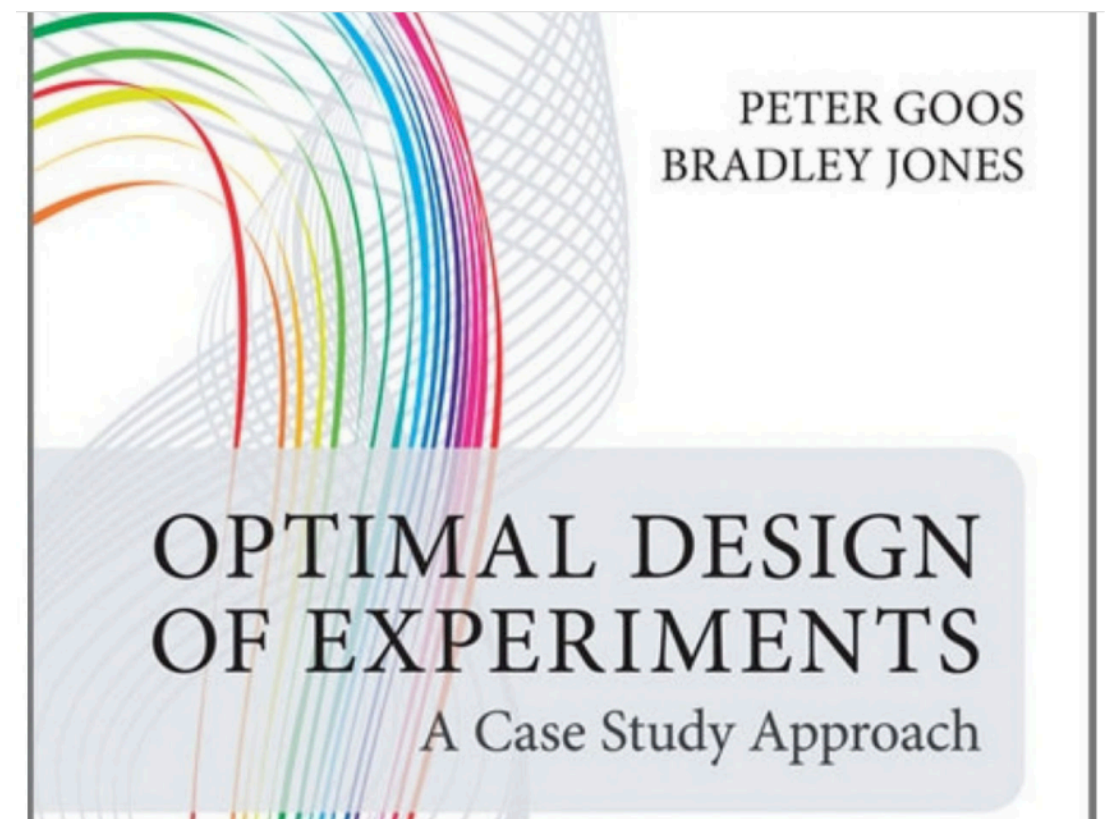# RECOMMENDED READING

▸ 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:

PETER GOOS
BRADLEY JONES

OPTIMAL DESIGN
OF EXPERIMENTS
A Case Study Approach

▸ https://www.jmp.com/en_us/applications/design-of-experiments.html

THANK YOU

FOR

LISTENING!