

WILLIAM BAUM

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?

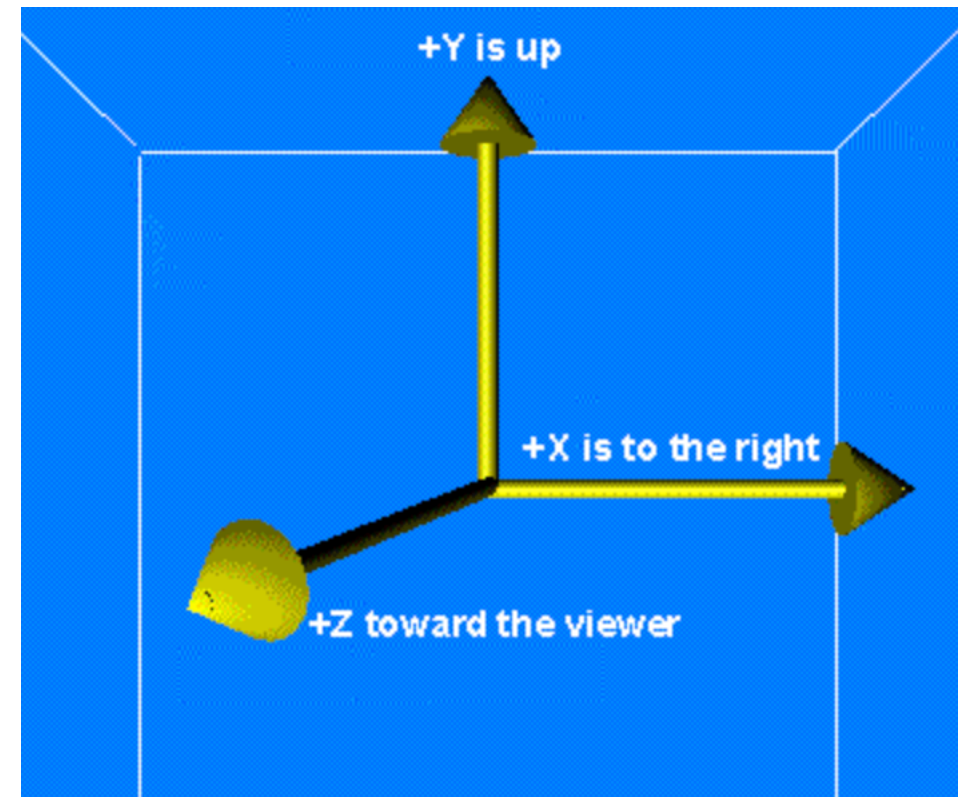


DESIGN OF
EXPERIMENTS

**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.
- ▶ 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.



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

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					
		③ Main Effects			④ Interactions		
		A	B	C	D (A-B)	E (A-C)	F (B-C)
② T e s t s	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

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

- ▶ 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>

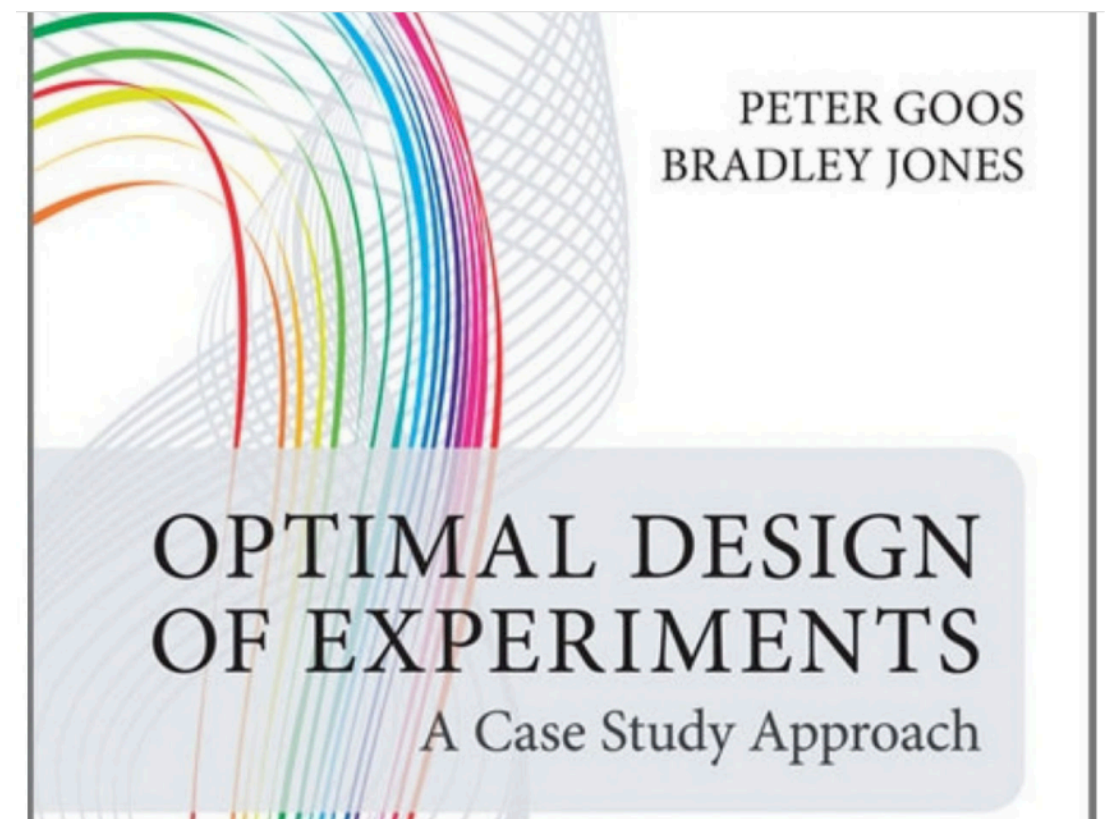
RECOMMENDED READING

- ▶ 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





THANK YOU
FOR
LISTENING!

