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 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

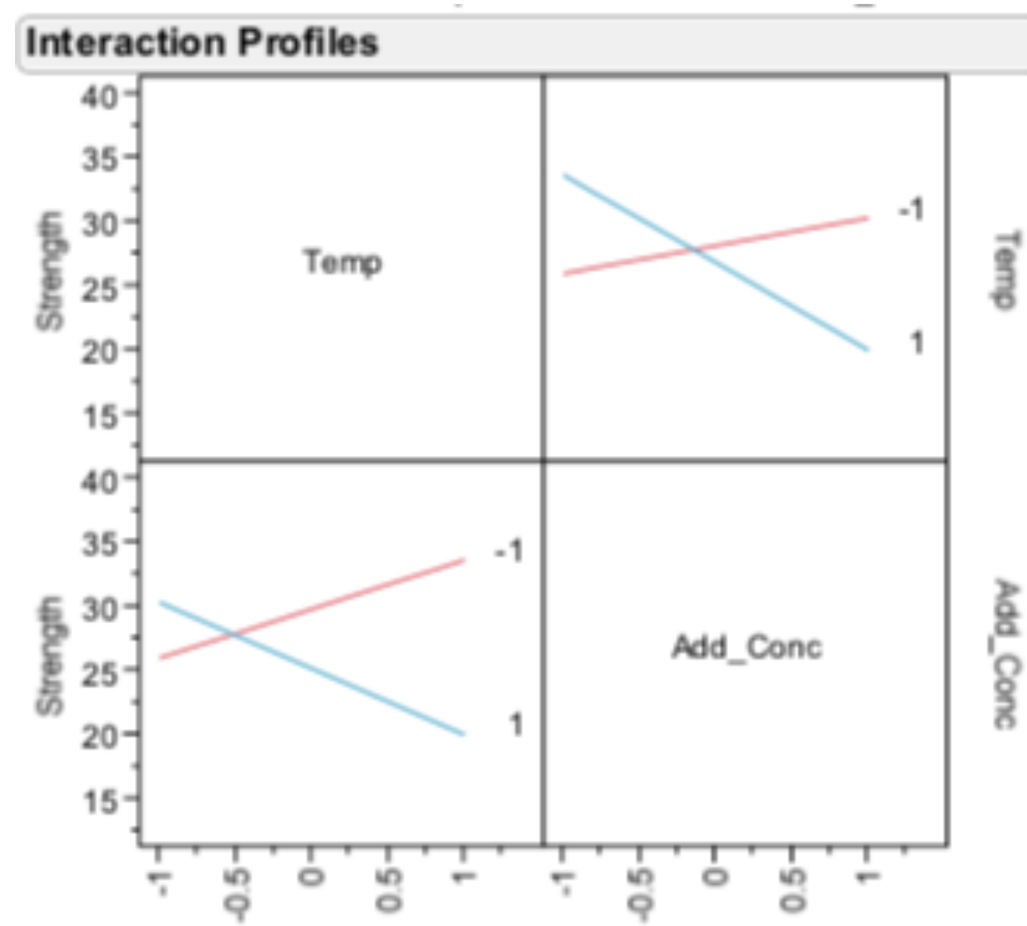
THE UNDERLYING STRUCTURE

CHARACTERISTICS OF DOE

- DOE systematically changes multiple input settings, simultaneously
- Allows for the estimation of main and interaction effects
- Systematic manipulation leads to better inference regarding *phenomenological causality* (literally, what happens to an outcome when you change input settings), compared with models based solely on observational data.
- Designs may be modified to incorporate and estimate covariates, as well as account for the difficulty in changing the settings of specific input factors.

ORTHOGONAL DESIGN – WHY IS THIS IMPORTANT IN DOE?

- DOE provides a system to produce designs with optimal efficiency by creating orthogonal, or near-orthogonal designs.
- Creates an efficient way to Estimate interaction effects on the full range of possible values of input factors.



Phillip Ramsey, PhD

- "The nonparallel lines in the interaction plot confirm that Temp and Add_Conc interact strongly. The impact of Temp on Strength depends on the setting of Add_Conc and vise versa."

INTERACTION EFFECTS – CONTINUOUS OUTCOME

Cats!	Inputs		Outcome
Runs	Male	Female	Kittens
1	-	+	0
2	+	-	0
3	+	+	8

http://www.guibingzhuche.com/free-cat-vector

INTERACTION EFFECTS – CONTINUOUS OUTCOME

	Inputs		Outcome
Runs	Brush	Floss	Cavities
1	+	+	0
2	+	-	2
3	-	+	3
4	-	-	5

https://shopcraftables.com/Free-Tooth--SVG-Cut-File

INTERACTION EFFECTS: THREE-WAY INTERACTIONS

- Fire
  - Heat
  - Oxygen
  - Fuel

	Inputs			Outcome
Runs	**Temp**	**Oxygen**	**Fuel**	**Fire**
1	-	+	+	No
2	+	+	-	No
3	+	-	+	No
4	+	+	+	Yes

http://clipart-library.com/free-fire-images.html

ESTIMATING VARIABILITY AND QUADRATIC EFFECTS

- Center-points help in detecting non-linear or quadratic effects on continuous outcomes.
- Replication (repeating runs of the same configuration) - helps to estimate how variability in a process effects outcomes.

OPTIMAL DESIGN

BUDGET SENSITIVE

① Factor Assignment

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

Design Of Experiments (DOE)

- 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, alone, when you can do so for multiple responses at once?

  Often, more than one outcome is important…

- You can do it easily with Multiple Response Optimization [MRO]!

MULTIPLE RESPONSE OPTIMIZATION

- 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: Serves to optimize all DFs, together, simultaneously to inform a final decision on input settings
  - The Full Details: The R package by Max Kuhn
    https://cran.r-project.org/web/packages/desirability/vignettes/desirability.pdf

DESIGN OF EXPERIMENTS

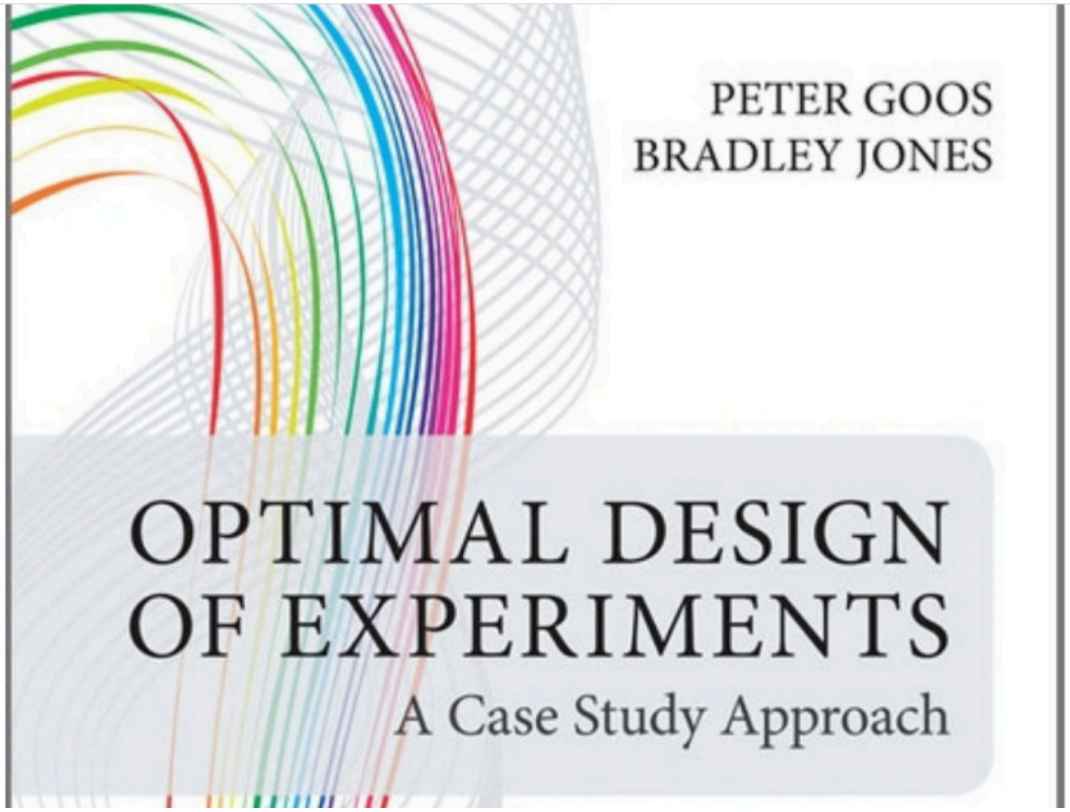
READING & RESOURCES

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 Desirability package, by Max Kuhn: 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!