Panel on Design of Experiment

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A typical Scientific Study

- Objective of the Study
- Set up Hypothesis
  (or set up underlying model, if possible)
- Prior knowledge
  - Cost (which determines the run size);
  - Number of variables, etc.
  - Not necessary in "functional" form
    (Prior distribution)
- Design of experiment
- Analysis, and etc...Decision making

The Role of Experiment Design When

- When we have extremely well understanding about the problem, or
- When we have only a vague understanding about the problem, or
- Somewhere in between

Design Objectives

- Treatment Comparison
- Screening
- Model Building
- Parameter Estimation
- Optimization
- Prediction
- Confirmation
- Discovery (Random Shot)
- etc.

Example: Screening Experiments

- Random Shot
- Group Screening
- Supersaturated Design
- One-At-A-Time Experiment
- Latin Hypercube
- Uniform Design
- etc.

k is large
n is small
p is small ($<<k$)

Which is the "best" (Optimal)?

Some fundamental Issues

- Design comes before data analysis.
  - Design with or without Model
- What can randomization do for you?
  - Design without randomization
- What can orthogonality do you ?
  - Non-orthogonal design

Design Criteria

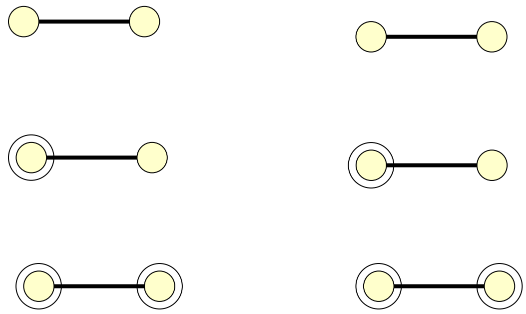
- Combinatorics Design
  - Orthogonality
  - Uniformity
  - Resolution
  - Aberration
  - Projection
  - Clear factors
- Optimal Design
  - Information matrix
  - D-optimality (eigenvalue type alphabetic optimalities)
  - Pukelsheim (1993) book
  - Kiefer's original work

Required Information

- Combinatorics Design
  - Number of factors (k)
  - Number of runs (n)
  - Number of Levels
  - Limitation on n
    - $n=4t$ (HM)
    - certain relationship between n and k (e.g., $n=2^{k-p}$)
  - Orthogonality
- Optimal Design
  - Number of factors (k)
  - Number of runs (n)
  - The underlying model
  - Optimality Criterion

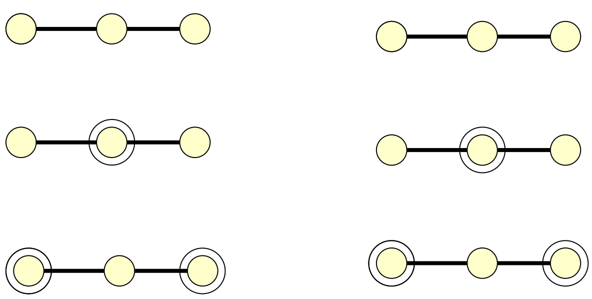
Some Examples in d=1 Dimension
First-Order Model

	Two-Level Factorial	D-optimal Design
$n=2$		
$n=3$		
$n=4$		



Some Examples in d=1 Dimension
Second-Order Model

	Three-Level Factorial	D-optimal Design
$n=3$		
$n=4$		
$n=5$		



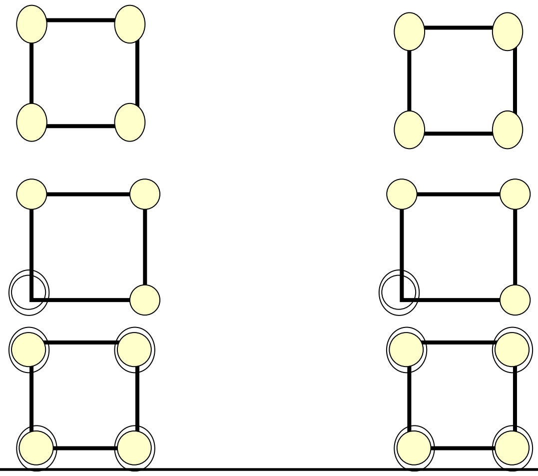
Some Examples in d=2 Dimension
First-Order Model

Two-Level Factorial | D-optimal Design

$n=4$

$n=5$

$n=8$

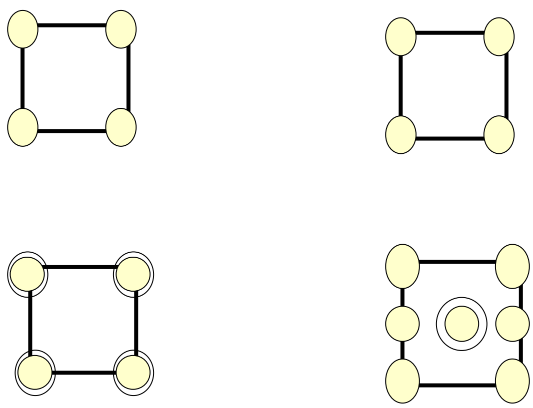


Some Examples in d=2 Dimension
Second-Order Model

Two-Level Factorial | D-optimal Design

$n=4$

$n=8$



D-optimal Designs in higher degree (d-1 Dimension)

Pukelsheim (1993)

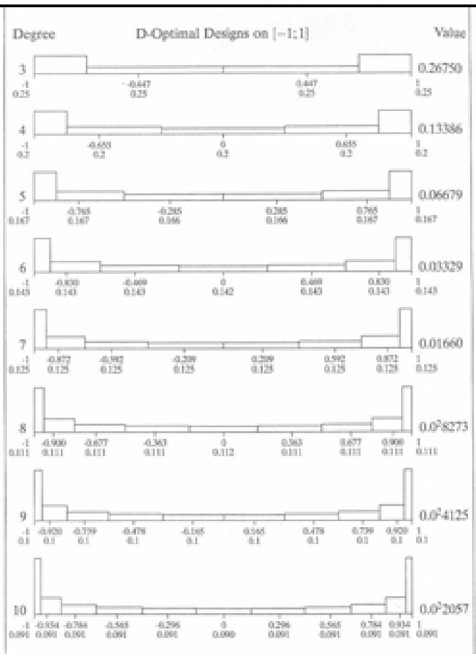


EXHIBIT 9.2 Polynomial fits over [−1;1]: ϕ_0-optimal designs τ_0^d for θ in T. Left: degree d of the fitted polynomial. Middle: support points and weights of τ_0^d, and a histogram representation. Right: optimal value $v_d(\phi_0)$ of the determinant criterion.

Did you know:
In many "practical" cases,
they are identical!!!

Design of Experiment

- Model (M)
- Number of Factors (*k*)
- Number of runs (*n*)

Models

Statistics vs. Engineering Models

$$y = f(x, \theta) + \varepsilon$$

Statistical Model

$$y = \beta_0 + \Sigma\beta_i x_i + \Sigma\beta_{ij} x_i x_j + \varepsilon$$

A Typical Engineering Model (page 1 of 3, in Liao and Wang, 1995)

$$
\begin{aligned}
&\rho_b A_b \frac{\partial^2 w}{\partial t^2} + E_b I_b \frac{\partial^4 w}{\partial x^4} \\
&+\{(\rho_s A_s + \rho_c A_c)\frac{\partial^2 w}{\partial t^2} + \rho_s A_s (\frac{t_b + t_s}{2})(\frac{\partial^3 u_b}{\partial x \partial t^2} - \frac{t_b + t_s}{2}\frac{\partial^4 w}{\partial x^2 \partial t^2} + \frac{t_s}{2}\frac{\partial^3 \beta}{\partial x \partial t^2}) \\
&+\rho_c A_c a(\frac{\partial^3 u_b}{\partial x \partial t^2} - a\frac{\partial^4 w}{\partial x^2 \partial t^2} + t_s \frac{\partial^3 \beta}{\partial x \partial t^2}) + C_{11}^{D} I_c \frac{\partial^4 w}{\partial x^4} - E_c A_c a(\frac{\partial^3 u_b}{\partial x^3} - a\frac{\partial^4 w}{\partial x^4} + t_s \frac{\partial^3 \beta}{\partial x^3})\}[H(x - x_1) - H(x - x_2)] \\
&+\{\rho_s A_s (\frac{t_b + t_s}{2})(\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b + t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c a(\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \\
&+2C_{11}^{D} I_c \frac{\partial^3 w}{\partial x^3} - 2E_c A_c a(\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})\}[\delta(x - x_1) - \delta(x - x_2)] \\
&+\{C_{11}^{D} I_c \frac{\partial^2 w}{\partial x^2} - E_c A_c a(\frac{\partial u_b}{\partial x} - a\frac{\partial^2 w}{\partial x^2} + t_s \frac{\partial \beta}{\partial x}) + b d_{31} E_c a V(t)\}[\delta'(x - x_1) - \delta'(x - x_2)] = f(x,t)
\end{aligned}
\tag{1}
$$

$$
\begin{aligned}
&\rho_b A_b \frac{\partial^2 u_b}{\partial t^2} - E_b A_b \frac{\partial^2 u_b}{\partial x^2} \\
&+\{\rho_s A_s (\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b + t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c (\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \\
&-E_c A_c (\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})\}[H(x - x_1) - H(x - x_2)] \\
&+\{-E_c A_c (\frac{\partial u_b}{\partial x} - a\frac{\partial^2 w}{\partial x^2} + t_s \frac{\partial \beta}{\partial x}) + b d_{31} E_c V(t)\}[\delta(x - x_1) - \delta(x - x_2)] = 0
\end{aligned}
\tag{2}
$$

$$
\begin{aligned}
&[\rho_s A_s \frac{t_s}{2}(\frac{\partial^2 u_b}{\partial t^2} - \frac{t_b + t_s}{2}\frac{\partial^3 w}{\partial x \partial t^2} + \frac{t_s}{2}\frac{\partial^2 \beta}{\partial t^2}) + \rho_c A_c t_s (\frac{\partial^2 u_b}{\partial t^2} - a\frac{\partial^3 w}{\partial x \partial t^2} + t_s \frac{\partial^2 \beta}{\partial t^2}) \\
&+A_s (G \cdot \beta) - E_c A_c t_s (\frac{\partial^2 u_b}{\partial x^2} - a\frac{\partial^3 w}{\partial x^3} + t_s \frac{\partial^2 \beta}{\partial x^2})][H(x - x_1) - H(x - x_2)]
\end{aligned}
\tag{3}
$$

Number of Factors (k)

- Agricultural Experiment vs
  Industrial Experiment
- Screening Design vs
  High-Level (Full) Factorial Design
- Grouping Design
- Textbook k=3 to 5
  Practical k=20 to 200 (to some 6000+)

What is the optimal number of runs (n)?

- As many as possible (n>30)
  - Typical Scientists (College of Science)
- $how me the Money
  - Project Manager (Business School)
- 1
  - Engineers—for confirmation only
- 0
  - Mathematical Statistician—We've proved it!

Summary: Design of Experiment

- ***Model is known***
  - Optimal design
  - Optimality Criteria
    (e.g., alphabetical optimalities)
- ***Model is unknown***
  (or is not completely known)
  - Bayesian Design
  - Robustness
  - Robustness Criterion
  - Representative Points

Optimal vs Robust

Some Minor Points

- Some solutions for Optimal Design may be involved with $i=\sqrt{-1}$
  which may not be easy to implement.
- *Rounding* may be sensitive for the optimality evaluation, although not much impact in practice
  —x=1.1234 vs x=1.1100.

DOE for Future Advanced Technology
(Partial List)

- Design for Quality (in FDA)
- Computer Experiment
  - Expensive simulation
  - Design with very large n
- MicroArray Experiment
  - Comments from Stan Young
- Split-Plot type Design
  - Hard-To-Change Variable etc.
- Nano-Technology Problem

How would optimal design fit here?

Where have all the Data gone?

- No need for data (Theoretical Development)
- Survey Sampling and Design of Experiment (Physical data collection)
- Computer Simulation (Experiment)
  - Statistical Simulation (Random Number Generation)
  - Engineering Simulation
- Data from Internet
  - On-line auction
  - Search Engine

Design of Experiment in Marketing and Social Studies:

where the "model" is not in mathematical functional form!!!
(Have a fun with HR people lately?)

Genetic Studies

- Model is completed unknown
- Classical (agricultural) designs are popular here—these are typically combinatorics designs.

Type of Designs

- Combinatorics Design
  - (Fractional) Factorial
  - Orthogonal Arrays
  - Latin Hypercube
  - Uniform Design
- Optimal Design (Bayesian Design)

- Middle Ground?
  - Chen, Lin and Tsai (2005)

Common Ground:

Conditional Optimal Design
by Chen, Lin & Tsai (2005)

- Use combinatroric design at the first stage (typically for screening and Steepest ascent)—model is not clear.
- When curvature is found and the second-order model is called for—model is known, use optimal design for additional experiments.
- Life is beautiful!!!

Practical & Theoretical

- Practical: We know how to make it work, but we don't know why.
- Theoretical: We know exactly why, but we don't know how to make it work.

- Now with Practical and Theoretical combined...

  It doesn't work and we don't know why!

Conclusion

- Every design has its own properties and values.

- There is more than one way for success.

- Those who can tell good advice from bad advice probably don't need any advice!

  For others, cook book is helpful.