CHAPTER 17

OPTIMAL DESIGN FOR EXPERIMENTAL INPUTS

• Organization of chapter in ISSO
  – Background
    • Motivation
    • Finite sample and asymptotic (continuous) designs
    • Precision matrix and $D$-optimality
  – Linear models
    • Connections to $D$-optimality
    • Key equivalence theorem
  – Response surface methods
  – Nonlinear models
Optimal Design in Simulation

• Two roles for experimental design in simulation
  – Building approximation to *existing* large-scale simulation via “metamodell”
  – Building simulation model itself

• Metamodels are “curve fits” that approximate simulation input/output
  – Usual form is low-order polynomial in the inputs; linear in parameters $\theta$
  – *Linear* design theory useful

• Building simulation model
  – Typically need *nonlinear* design theory

• Some terminology distinctions:
  – “*Factors*” (statistics term) $\rightarrow$ “*Inputs*” (modeling and simulation terms)
  – “*Levels*” $\rightarrow$ “*Values*”
  – “*Treatments*” $\rightarrow$ “*Runs*”
Unique Advantages of Design in Simulation

- Simulation experiments may be considered special case of general experiments
- Some unique benefits occur due to simulation structure
- Can control factors not generally controllable (e.g., arrival rates into network)
- Direct repeatability due to deterministic nature of random number generators
  - Variance reduction (CRNs, etc.) may be helpful
- Not necessary to randomize runs to avoid systematic variation due to inherent conditions
  - E.g., randomization in run order and input levels in biological experiment to reduce effects of change in ambient humidity in laboratory
  - In simulation, systematic effects can be eliminated since analyst controls nature
Design of Computer Experiments in Statistics

• There exists significant activity among statisticians for experimental design based on computer experiments
  – T. J. Santner et al. (2003), *The Design and Analysis of Computer Experiments*, Springer-Verlag
  – Etc.

• Above statistical work differs from experimental design with *Monte Carlo simulations*
  – Above work assumes *deterministic function evaluations* via computer (e.g., solution to complicated ODE)

• One implication of deterministic function evaluations: no need to replicate experiments for given set of inputs

• Contrasts with Monte Carlo, where replication provides variance reduction
General Optimal Design Formulation (Simulation or Non-Simulation)

- Assume model
  \[ z = h(\theta, x) + v , \]
  where \( x \) is an input we are trying to pick optimally

- Experimental design \( \xi \) consists of \( N \) specific input values \( x = \chi_i \) and proportions (weights) to these input values \( w_i : \)

\[ \xi \equiv \begin{pmatrix} \chi_1 & \chi_2 & \cdots & \chi_N \\ w_1 & w_2 & \cdots & w_N \end{pmatrix} \]

- **Finite-sample** design allocates \( n \geq N \) available measurements exactly; **asymptotic (continuous)** design allocates based on \( n \to \infty \)
**D-Optimal Criterion**

- Picking optimal design $\xi$ requires criterion for optimization.
- Most popular criterion is $D$-optimal measure.
- Let $\mathbf{M}(\theta, \xi)$ denote the “precision matrix” for an estimate of $\theta$ based on a design $\xi$.
  - $\mathbf{M}(\theta, \xi)$ is inverse of covariance matrix for estimate
  - $\mathbf{M}(\theta, \xi)$ is Fisher information matrix for estimate.
- $D$-optimal solution is
  \[ \xi^* = \arg \max_{\xi} \{ \det[\mathbf{M}(\theta, \xi)] \} \]
Equivalence Theorem

- Consider linear model
  \[ z_k = h_k^T \theta + v_k, \quad k = 1, 2, \ldots, n \]

- Prediction based on parameter estimate \( \hat{\theta}_n \) and "future" measurement vector \( h^T \) is
  \[ \hat{z} = h^T \hat{\theta}_n \]

- Kiefer-Wolfowitz equivalence theorem states:
  \[ D \text{-optimal solution for determining } \xi \text{ to be used in forming } \hat{\theta}_n \text{ is the same } \xi \text{ that minimizes the maximum variance of predictor } \hat{z} \]

- Useful in practical determination of optimal \( \xi \)
Variance Function as it Depends on Input: Optimal *Asymptotic* Design for Example 17.6 in *ISSO*
Orthogonal Designs

• With linear models, usually more than one solution is $D$-optimal
• Orthogonality is means of reducing number of solutions
• Orthogonality also introduces desirable secondary properties
  – Separates effects of input factors (avoids “aliasing”)
  – Makes estimates for elements of $\theta$ uncorrelated
• Orthogonal designs are not generally $D$-optimal; $D$-optimal designs are not generally orthogonal
  – However, some designs are both
• Classical factorial (“cubic”) designs are orthogonal (and often $D$-optimal)
Example Orthogonal Designs, $r = 2$ Factors

Cube ($2^r$ design)

Star ($2r$ design)
Example Orthogonal Designs, $r = 3$ Factors

Cube ($2^r$ design)

Star ($2r$ design)