Steps of RSM for Optimizing $x$

**Step 0 (Initialization)** Initial guess at optimal value of $x$.

**Step 1 (Collect data)** Collect responses $z$ from several $x$ values in neighborhood of current estimate of best $x$ value (can use experimental design).

**Step 2 (Fit model)** From the $x$, $z$ pairs in step 1, fit regression model in region around current best estimate of optimal $x$.

**Step 3 (Identify steepest descent path)** Based on response surface in step 2, estimate path of steepest descent in factor space.

**Step 4 (Follow steepest descent path)** Perform series of experiments at $x$ values along path of steepest descent until no additional improvement in $z$ response is obtained. This $x$ value represents new estimate of best vector of factor levels.

**Step 5 (Stop or return)** Go to step 1 and repeat process until final best factor level is obtained.
Nonlinear Design

• Assume model

\[ z = h(\theta, x) + \nu, \]

where \( \theta \) enters nonlinearly

• \( D \)-optimality remains dominant measure
  – Maximization of determinant of Fisher information matrix (from Chapter 13 of ISSO: \( \mathbf{F}_n(\theta, x) \) is Fisher information matrix based on \( n \) data points)

• Fundamental distinction from linear case is that \( D \)-optimal criterion depends on \( \theta \)

• Leads to conundrum:

Choosing \( x \) to best estimate \( \theta \), yet need to know \( \theta \) to determine \( x \)
Strategies for Coping with Dependence on $\theta$

- Assume nominal value of $\theta$ and develop an optimal design based on this fixed value.
- Sequential design strategy based on an iterated design and model fitting process.
- Bayesian strategy where a prior distribution is assigned to $\theta$, reflecting uncertainty in the knowledge of the true value of $\theta$. 

Sequential Approach for Parameter Estimation and Optimal Design

**Step 0 (Initialization)** Make initial guess at $\theta, \hat{\theta}_0$. Allocate $n_0$ measurements to initial design. Set $k = 0$ and $n = 0$.

**Step 1 (D-optimal maximization)** Given $X_n$, choose the $n_k$ inputs in $X = X_{nk}$ to maximize
\[
det[F_n(\hat{\theta}_n, X_n) + F_{nk}(\hat{\theta}_n, X)].
\]

**Step 2 (Update $\theta$ estimate)** Collect $n_k$ measurements based on inputs from step 1. Use measurements to update from $\hat{\theta}_n$ to $\hat{\theta}_{n+n_k}$.

**Step 3 (Stop or return)** Stop if the value of $\theta$ in step 2 is satisfactory. Else return to step 1 with the new $k$ set to the former $k + 1$ and the new $n$ set to the former $n + n_k$ (updated $X_n$ now includes inputs from step 1).
Comments on Sequential Design

• Note two optimization problems being solved: one for $\xi$, one for $\theta$

• Determine next $n_k$ input values (step 1) conditioned on current value of $\theta$
  – Each step analogous to nonlinear design with fixed (nominal) value of $\theta$

• “Full sequential” mode ($n_k = 1$) updates $\theta$ based on each new input–output pair $(x_k, z_k)$

• Can use stochastic approximation to update $\theta$:

\[
\hat{\theta}_{n+1} = \hat{\theta}_n - a_n Y_n (\hat{\theta}_n \mid z_{n+1}, x_{n+1})
\]

where

\[
Y_n (\theta \mid z_{n+1}, x_{n+1}) = \frac{1}{2} \frac{\partial}{\partial \theta} [z_{n+1} - h(\theta, x_{n+1})]^2
\]
Bayesian Design Strategy

• Assume prior distribution (density) for $\theta$, $p(\theta)$, reflecting uncertainty in the knowledge of the true value of $\theta$.
• There exist multiple versions of $D$-optimal criterion
• One possible $D$-optimal criterion:

$$E_{\theta}\left\{ \log \det [F_n(\theta, X)] \right\} = \int_{\Theta} \log \det [F_n(\theta, X)] p(\theta) d\theta$$

• Above criterion related to Shannon information
• While log transform makes no difference with fixed $\theta$, it does affect integral-based solution.
• To simplify integral, may be useful to choose discrete prior $p(\theta)$