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Response Surface Methodology (RSM)

☆ $E(y_{\tilde{x}}) = f(\tilde{x})$

☆ $\hat{y}_{\tilde{x}}$: predictors of $E(y_{\tilde{x}})$

⇓

$\sum \hat{\beta}_i g_i(\tilde{x})$

RSM

factorial design

C.P.

☆ RSM less concerns about ① effect orthogonality, ② effect aliasing, ③ identification of significant effect.

☆ RSM use fixed model ← already contain all important effects

$\hat{y}_{\tilde{x}} \longleftrightarrow \hat{\beta}_i$'s

more stable

meaning?

RSM

factorial designs

- Experimental study focusing on the relationship between the response and the input factors.

  (f)

- Common purposes in RSM:
  - Optimizing the response → find $\tilde{x}$ that maximize/minimize $E(y_{\tilde{x}})$
  - Mapping the response surface over a region of interest → predictor of $E(y_{\tilde{x}})$
- Sequential experimentation strategy for optimization

  ← Note: experimentation is a learning process.

- RSM is an effective tool especially when
  - input factors are quantitative ← why $f(\tilde{x})$ is called response surface.
  - there are only a few of input factors.

Ranitidine Experiment

- Consider an experiment to study three quantitative factors with up to 5 levels.

Table 1: Factors and Levels, Ranitidine Experiment

Factor	Levels
A. pH	2, 3.42, 5.5, 7.58, 9
B. voltage (kV)	9.9, 14, 20, 26, 30.1
C. α-CD (mM)	0, 2, 5, 8, 10

← center point

- The design matrix and the data are given on the next page. The design differs from 2^{k-p} design in two respects :
  - 6 replicates at the center,
  - 6 runs along the three axes.

It belongs to the class of *central composite designs* (CCD).

Ranitidine Experiment

Table 2: Design Matrix and Response Data

	Factor				
Run	*A*	*B*	*C*	CEF	ln CEF
1	−1	−1	−1	17.293	2.850
2	1	−1	−1	45.488	3.817
3	−1	1	−1	10.311	2.333
4	1	1	−1	11757.084	9.372
5	−1	−1	1	16.942	2.830
6	1	−1	1	25.400	3.235
7	−1	1	1	31697.199	10.364
8	1	1	1	12039.201	9.396
9	0	0	−1.67	7.474	2.011
10	0	0	1.67	6.312	1.842
11	0	−1.68	0	11.145	2.411
12	0	1.68	0	6.664	1.897
13	−1.68	0	0	16548.749	9.714
14	1.68	0	0	26351.811	10.179
15	0	0	0	9.854	2.288
16	0	0	0	9.606	2.262
17	0	0	0	8.863	2.182
18	0	0	0	8.783	2.173
19	0	0	0	8.013	2.081
20	0	0	0	8.059	2.087

Ranitidine Experiment

The CCD has three parts ← each part appear for different purposes.

(1) *cube* (or corner) points, (2) *axial* (or star) points, (3) *center* points.

(•) (×) (o)

a second-order design

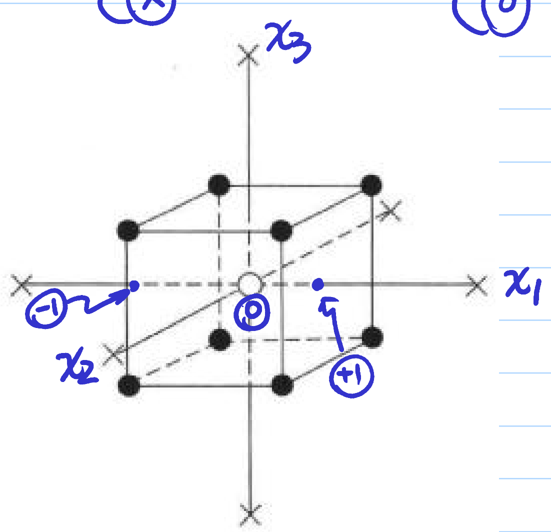


Figure 1: A Central Composite Design in Three Dimensions [cube point (dot), star point (cross), center point (circle)].

v **Reading**: textbook, 10.1

Sequential Nature of RSM

- Basic concepts
  - For a process/system involving a response y and *input factors* $X_1, \ldots, X_k$, model their relationship by

$E(y_x)$

$$y = f(X_1, \ldots, X_k) + \varepsilon,$$

true response surface

Hint: Taylor expansion

where f is unknown.

  - *Locally* approximate f by

$\forall \varepsilon > 0, \exists \delta > 0$. s.t. when $\|x - x_0\| < \delta$
$|f(x) - (k\text{th-order polynomial of } x)| < \varepsilon$

$$f(X_1, \ldots, X_k) \approx \sum_{i=1}^{m} \beta_i \cdot g_i(X_1, \ldots, X_k)$$

often use polynomial terms of $x_1, \ldots, x_k$.

where β_i's: unknown parameters, and g_i's: known functions of $X_1, \ldots, X_k$

  - Conduct experiments and collect data to estimate β_i's
  - Use *fitted response surface* $\hat{f}$ to understand f:

β_i's: tools for approximation purpose, may not concern whether β_i's carry physical interpretation.

$$\hat{f} = \sum_{i=1}^{m} \hat{\beta}_i \cdot g_i(X_1, \ldots, X_k) \longrightarrow f$$

Sequential Nature of RSM

- Sequential experimentation to maximize/minimize the response or to achieve a desired value of the response: Find x s.t. $E(y_x) = C$.

RSM is effective when # of factors is small.

factor screening

1. **Screening Experiment :** When many variables are considered, some are likely to be inert. Use *a 2^{k-p} design or an OA.* identify important factors

   Why? efficiency consideration

   e.g. A, B, C, ..., I, J (10 factors)
   more important.
   \$1000, equally distributed to 10 factor. / use 20% to identify A & B. 80% to study effects of A&B

   (c.f.) information ↓ identify important effects. information ↑
   $y \sim A+B$
   $y \sim A+B+AB$
   $y \sim A+AB$
   → important factors: A & B.

2. Once a small number of important factors is identified, if the experimental region is far from the optimum (examined by **curvature check**), use the **first-order model**

   1st-order design (2-level)
   ① FFD (resolution ≥ III)
   ② orthogonal M.E. plan
   ③ orthogonal array

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon, \quad (1)$$

to fit the data.

Sequential Nature of RSM

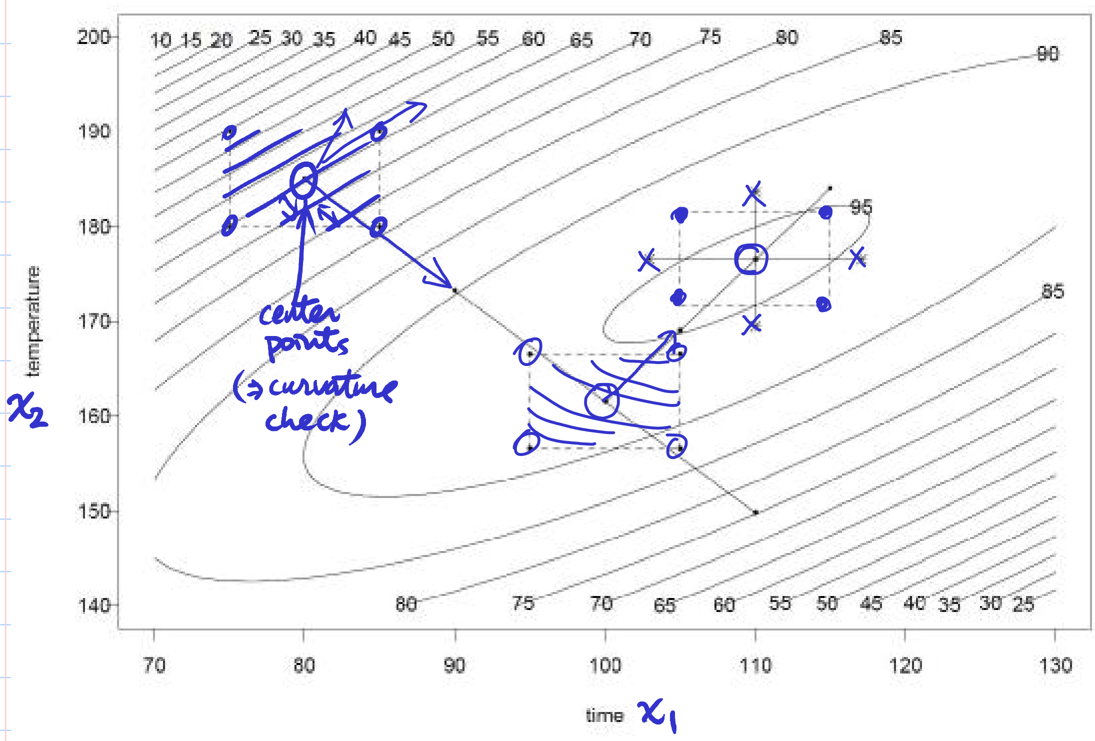
3. Based on the fitted first-order model, find the steepest ascent direction and perform a search along this direction (called **steepest ascent search**).
   - Steps 2 and 3 may be repeated until reaching the optimum region (e.g. peak of the surface).
   - Alternative to steps 2 and 3: **rectangular grid search**
4. To capture the curvature effects, use a **second-order design** (like the central composite design). Fit a **second-order model**

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i<j}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I) \qquad (2)$$

to data. Use the fitted model (with insignificant terms dropped) to do *contour plots* and find the *optimum* conditions.

A graphical illustration of these steps is given on next page.

Sequential Exploration of Response Surface



v Reading: textbook, 10.2