Center Points and Curvature Check

↳ 2-level factor → 3-level factor.

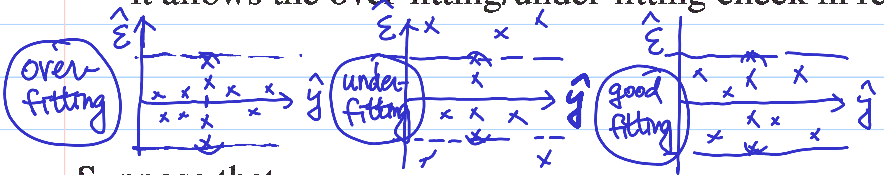
- Purposes of adding $\boxed{\textit{replicated}}$ center points to a 2-level first-order experiment

  ↳ pure error estimate ↖ using 2^{k-p} or OA

  - it allows the check of the overall curvature effect,
  - it provides an unbiased estimate of the process error variance

    Note constant variance assumption → $\hat{\sigma}^2$ → can do t-test for saturated 2^{k-p}

  - it allows the over-fitting/under-fitting check in residual plot



- Suppose that

  i.e. resolution ≥ 3 strength ≥ 2

  - the first-order experiment is based on a 2-level $\boxed{\text{orthogonal design}}$ with run size n_f, and

    ↖ projection onto any 2 factors ⇒ full 2^2 design.

  - n_c center point runs are added to the first-order experiment.

Center Points and Curvature Check

- Let $\bar{y}_f$ = sample average over factorial runs with level ± 1, ← $\sum_{\underset{\sim}{x} \in D} y_{\underset{\sim}{x}} / n_f$

  $\bar{y}_c$ = sample average at n_c center points with level 0 ← $\sum_{\underset{\sim}{x}=0} y_{\underset{\sim}{x}} / n_c$

- Under the second-order model

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

may be aliased

$E\left(\sum_{\underset{\sim}{x} \in D} y_{\underset{\sim}{x}}\right) / n_f = \sum_{\underset{\sim}{x} \in D} E(y_{\underset{\sim}{x}}) / n_f$

$E(y_{\underset{\sim}{x}=0})$

$\sum_{\underset{\sim}{x} \in D} x_i = 0, \sum_{\underset{\sim}{x} \in D} x_i x_j = 0, \sum_{\underset{\sim}{x} \in D} x_i^2 = n_f$

  - $E(\bar{y}_c) = \beta_0$,
  - $E(\bar{y}_f) = \beta_0 + \sum_{i=1}^{k} \beta_{ii}$,
  - $E(\bar{y}_f - \bar{y}_c) = \sum_{i=1}^{k} \beta_{ii}$, and
  - $Var(\bar{y}_f - \bar{y}_c) = \sigma^2 (\frac{1}{n_f} + \frac{1}{n_c})$.

fitted model.

$y \sim \beta_0 + \{x_i\text{'s}, x_i x_j\text{'s estimable model}\} + \underbrace{(\beta_{11} + \cdots + \beta_{kk})}_{= \beta^*} x_i^2 + \varepsilon$

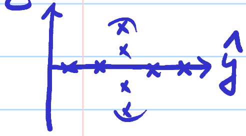
- *overall curvature* parameter: $\beta_{11} + \cdots + \beta_{kk}$ ← β^*
  - In using the overall curvature to measure the curvature effects, it is possible that some of the large β_{ii} cancel each other, thus yielding a very small $\sum_{i=1}^{k} \beta_{ii}$.

    LN p.3-29.

  - This rarely occurs unless exp'tal region near a $\boxed{\text{saddle point}}$ of the f.

Center Points and Curvature Check

$\hat{\varepsilon}$



- To test the hypotheses

$$H_0 : \beta_{11} + \cdots + \beta_{kk} = 0 \text{ v.s. } H_a : \beta_{11} + \cdots + \beta_{kk} \neq 0$$

we can use $\bar{y}_f - \bar{y}_c$.

- Reject H_0 at level α if

Same as the $\hat{\sigma}^2$ under the LM in LNp.3-10 if # of $\{\beta_0, \beta_i\text{'s}, \beta_{ij}\} = n_f$

indep

$$\frac{|\bar{y}_f - \bar{y}_c|}{s\sqrt{\frac{1}{n_f} + \frac{1}{n_c}}} > t_{\boxed{n_c-1}, \frac{\alpha}{2}}$$

where s^2= sample variance based on n_c center runs is used to estimate σ^2.

$\sum_{x=0} (y_x - \bar{y}_c)^2 / n_c - 1$

move to different exp'tal region

- If the curvature check is not significant the search may continue with the use of another first-order exeriment and steepest ascent. Otherwise, it should be swithched to a second-order experiment.

stay in the original exp'tal region.

Center Points and Curvature Check

orthogonal design

sum $x_i = 0$ sum $x_i x_j = 0$ sum $x_i^2 = n_f$

identical columns (they are aliased)

- Justification from regression analysis:

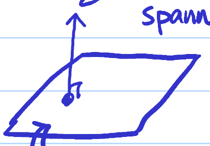
Design matrix   model matrix

$$\begin{array}{c|ccc|c|ccc|ccc|ccc}
 & x_1 & \cdots & x_k & \mathbb{1} & x_1 & \cdots & x_k & x_1x_2 & \cdots & x_{k-1}x_k & x_1^2 & \cdots & x_k^2 \\
n_f & +1 & & +1 & 1 & +1 & & +1 & & & & +1 & & +1 \\
 & +1 & & -1 & 1 & +1 & & -1 & & +1/-1 & & +1 & & +1 \\
 & \vdots & & \vdots & \vdots & \vdots & & \vdots & & & & \vdots & & \vdots \\
 & -1 & & -1 & 1 & -1 & & -1 & & & & +1 & & +1 \\
n_c & 0 & \cdots & 0 & 1 & 0 & & 0 & 0 & & 0 & 0 & & 0 \\
 & 0 & \cdots & 0 & 1 & 0 & & 0 & 0 & & 0 & 0 & & 0
\end{array}$$

X_f

$X_f^T X_f$ is nonsingular

2-dim space spanned by $\mathbb{1}$ & x_i^2



space spanned by $\{x_i\text{'s}, x_ix_j\}$

$Y = X\beta + \varepsilon$

$$X = \left[\begin{array}{c|cc} X_f & \mathbb{1} & x_i^2 \\ \underset{\sim}{0} & & \end{array}\right]$$

Z β_0 β^*

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}^* \end{bmatrix} = (Z^TZ)^{-1}Z^TY \rightarrow Z^TZ = \begin{bmatrix} n_c+n_f & n_f \\ n_f & n_f \end{bmatrix}$$

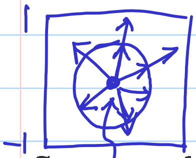
$$(Z^TZ)^{-1} = \begin{bmatrix} 1/n_c & -1/n_c \\ -1/n_c & \frac{n_c+n_f}{n_cn_f} \end{bmatrix} \propto Var(\hat{\beta}^*)$$

Least square give same estimate of β^*, but t-tests could be different

$$(Z^TZ)^{-1}\underbrace{Z^TY}_{=\begin{bmatrix} \sum_{x\in D} y_x + \sum_{x=0} y_x \\ \sum_{x\in D} y_x \end{bmatrix}} = \left[-\frac{\sum_{x\in D} y_x + \sum_{x=0} y_x}{n_c} + \left(\frac{1}{n_c} + \frac{1}{n_f}\right)\sum_{x\in D} y_x \right]$$

$$= \frac{\sum_{x\in D} y_x}{n_f} - \frac{\sum_{x=0} y_x}{n_c} = \bar{y}_f - \bar{y}_c$$

v **Reading**: textbook, 10.3.1



Steepest Ascent Search

fixed

$\underset{\sim}{x_0} \to \underset{\sim}{x_0} + \underset{\sim}{\Delta}$, where $\|\Delta\|^2 = d$

Q: What $\underset{\sim}{\Delta}$ cause largest increase/decrease on $\hat{y}$ under the model?

- Suppose the fitted model is

$\underset{\sim}{x_0}$

$x_i x_j$'s not significant
x_i^2's : :

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$$

- Taking the partial derivative of $\hat{y}$ with respect to x_i

$$\frac{\partial \hat{y}}{\partial x_i} = \hat{\beta}_i, \quad i = 1, \ldots, k.$$

$\max_{\underset{\sim}{\Delta}} \hat{y}(\underset{\sim}{x_0}+\underset{\sim}{\Delta}) - \hat{y}(\underset{\sim}{x_0}) = \sum \hat{\beta}_i \Delta_i$

subject to. $\|\Delta\|^2 = d$

Lagrange method

- The **steepest ascent** direction (for maximization) is

$$\lambda \cdot (\hat{\beta}_1, \ldots, \hat{\beta}_k), \quad \lambda > 0,$$

$\Rightarrow \max_{\underset{\sim}{\Delta}} \sum \hat{\beta}_i \Delta_i + \lambda(\|\Delta\|^2 - d) \equiv t(\underset{\sim}{\Delta}, \lambda)$, $\|\Delta\|^2 = \sum \Delta_i^2$

and the **steepest descent** direction (for minimization) is $\frac{\partial t}{\partial \Delta_i} = \hat{\beta}_i + 2\lambda\Delta_i = 0$

$$\lambda \cdot (\hat{\beta}_1, \ldots, \hat{\beta}_k), \quad \lambda < 0.$$

$\Rightarrow \Delta_i \propto \hat{\beta}_i$

Steepest Ascent Search

- The search for a higher (lower) response continues by
  - drawing a line from the center point of the design in the steepest ascent (descent) direction
  - performing $\boxed{\text{several runs}}$ along the steepest ascent (descent) path
  - taking the location on the path where a maximum (minimum) response is observed as the center point for the next experiment
- The design for the next experiment is again a first-order design plus some center runs.

Note1: the linear approximation (first-order fitted model) to the unknown true response is adequate in exp'tal region or region not far away the exp'tal region.

Note2: What if we change coding of effects, can we still get similar/same result? $\to$ RSM more interested in $\hat{y}$, not $\hat{\beta}$.

Illustrated Initial First-Order Experiment

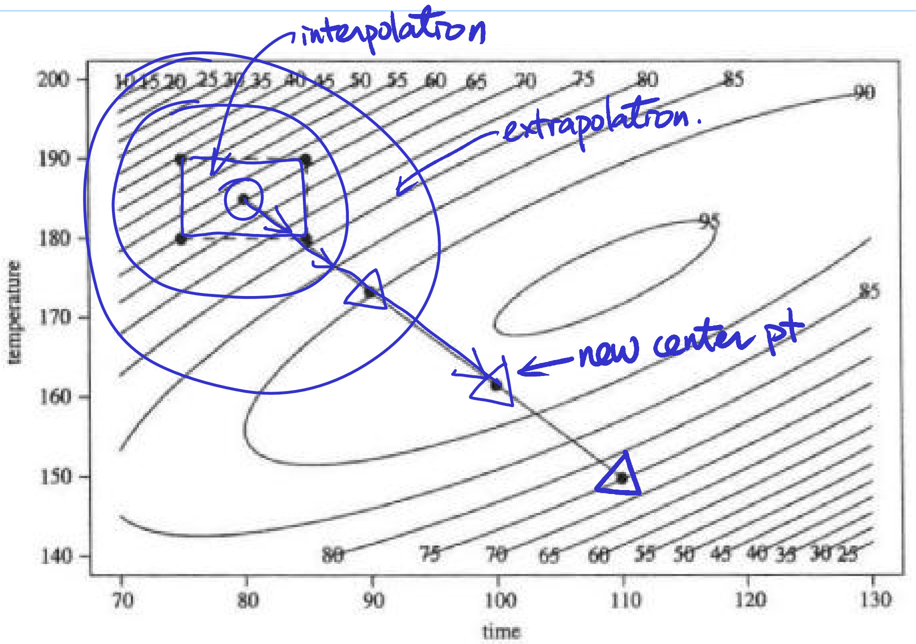


Figure 3: First-order experiment with steepest ascent

Illustrated Initial First-Order Experiment

Table 3: Design Matrix and Yield Data for First-Order Design

	Factor		
Run	Time	Temperature	Yield
1	−1 75min	180°C −1	65.60
2	−1 75min	190°C 1	45.59
3	1 85min	180°C −1	78.72
4	1 85min	190°C 1	62.96
5	0 80min	185°C 0	64.78
6	0 80min	185°C 0	64.33
7	2	2(-1.173)	89.73
8	4	4(-1.173)	93.04
9	6	6(-1.173)	75.06

2 level full factorial, can be used to estimate ~~x_i's &~~ x_1, x_2, x_1x_2

2-level design + center pt.

1st-order fitted model still work.

Illustrated Initial First-Order Experiment

- Model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + (\beta_{11} + \beta_{22}) x_1^2,$$

Table 4: Least Square Estimates, Standard Errors, t Statistics and p-values, Initial First-Order Experiment

1st-order model is OK. move to a new exptal region.

$n_f = 4$. # of $\{\beta_0, \beta_1, \beta_2, \beta_{12}\}$ $= 4$

$\hat{\sigma}^2 = s_0^2$

Effect	Estimate	Standard Error	t	p-value
intercept	64.5550	0.2250	286.91	0.00
β_1	7.6225	0.1591	47.91	0.01
β_2	-8.9425	0.1591	-56.21	0.01
β_{12}	1.0625	0.1591	6.68	0.09
$\beta_{11} + \beta_{22}$	-1.3375	0.2756	-4.85	0.13

not significant

curvature check.

Illustrated Steepest Ascent Search

$\hat{\beta}_1$ $\hat{\beta}_2$

- Steepest ascent direction: $(7.622, -8.942)$ or equivalently, $(1, -1.173)$

why not 1 unit?

- Increasing time in steps of 2 units (10 minutes) is used because a step of 1 unit would give a point near the southeast corner of the first order design
- The results for three steps appear as runs 7-9 in Table 3.
- Because run 8 (time=4, temperature=$4(-1.173)$) correspond to the maximum yield along the path, they would be a good center point for the next experiment
- A first-order experiment can be run as indicated by runs 1-6 in Table 5.

Illustrated Steepest Ascent Search

Table 5: Design Matrix and Yield Data for Second-Order Design

Run	Factor Time	Temperature	Yield
1	−1	−1	91.21
2	−1	1	94.17
3	1	−1	87.46
4	1	1	94.38
5	0	0	93.04
6	0	0	93.06
7	−1.41	0	93.56
8	1.41	0	91.17
9	0	−1.41	88.74
10	0	1.41	95.08

2-level design + center pts.

axial pts

$x_1^2 = x_2^2$

$x_1^2 \neq x_2^2$

Illustrated Second-Order Experiment

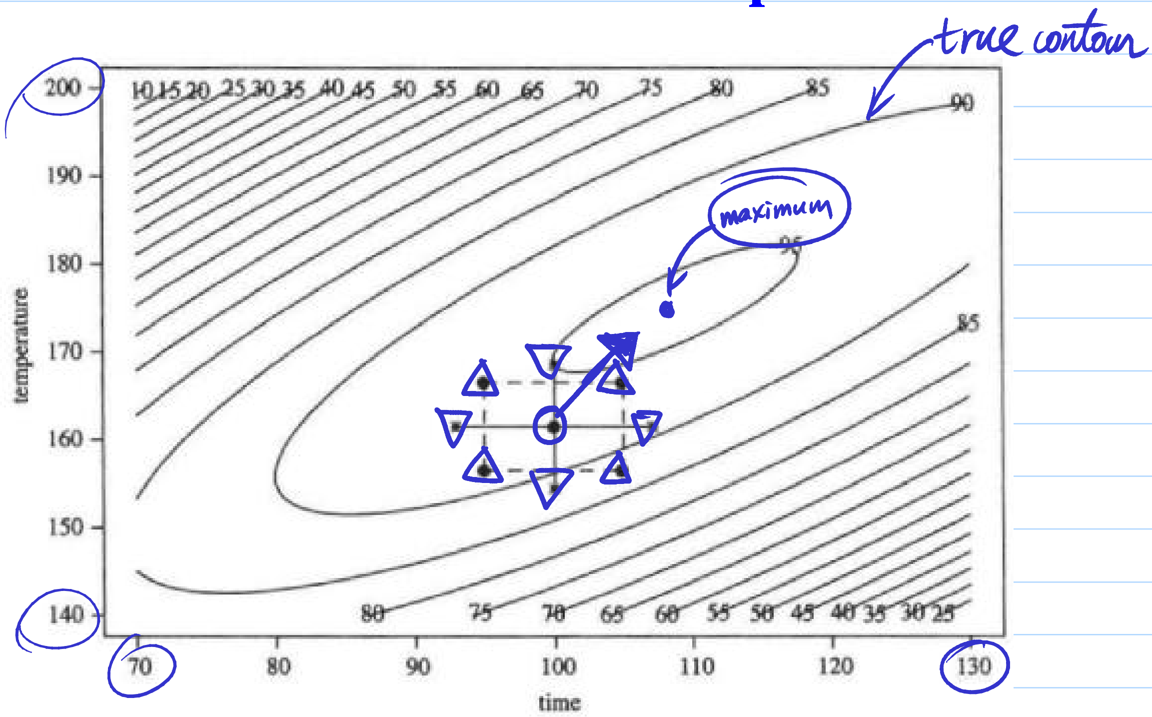


Figure 4: Second-order experiment

Illustrated Second-Order Experiment

Table 6: Least Square Estimates, Standard Errors, t Statistics and p-values for Follow-up First-Order Experiment

fitting 1st-order model is not enough

c.f. $\hat{\beta}_1$ & $\hat{\beta}_2$ in Table 4 (LN p.3-17)

Effect	Estimate	Standard Error	t	p-value
intercept	93.0500	0.0100	9305.00	0.000
β_1	-0.8850	0.0071	-125.17	0.005
β_2	2.4700	0.0071	349.31	0.002
β_{12}	0.9900	0.0071	140.01	0.005
$\beta_{11}+\beta_{22}$	-1.2450	0.0122	-101.65	0.006

significant

curvature check.

Table 7: Least Square Estimates, Standard Errors, t Statistics and p-values for Second-Order Experiment

+

Effect	Estimate	Standard Error	t	p-value
intercept	93.0500	0.2028	458.90	0.000
β_1	-0.8650	0.1014	-8.53	0.001
β_2	2.3558	0.1014	23.24	0.000
β_{12}	0.9900	0.1434	6.90	0.002
β_{11}	-0.4256	0.1341	-3.17	0.034
β_{22}	-0.6531	0.1341	-4.87	0.008

significant.

Illustrated Second-Order Experiment

- The results in Table 6 indicate that
  - there are significant interaction and curvature effects
  - the first-order design should be augmented to a $\boxed{\text{second-order design}}$

dealias $x_1^2 = x_2^2 = \cdots = x_k^2$

e.g. CCD

- The axial points of a CCD (runs 7-10 in Table 5) are performed
- The results of fitting a second-order model is given in Table 7. Fitted response surface model:

$$\hat{y} = 93.05 - 0.87x_1 + 2.36x_2 + 0.99x_1x_2 - 0.43x_1^2 - 0.65x_2^2.$$

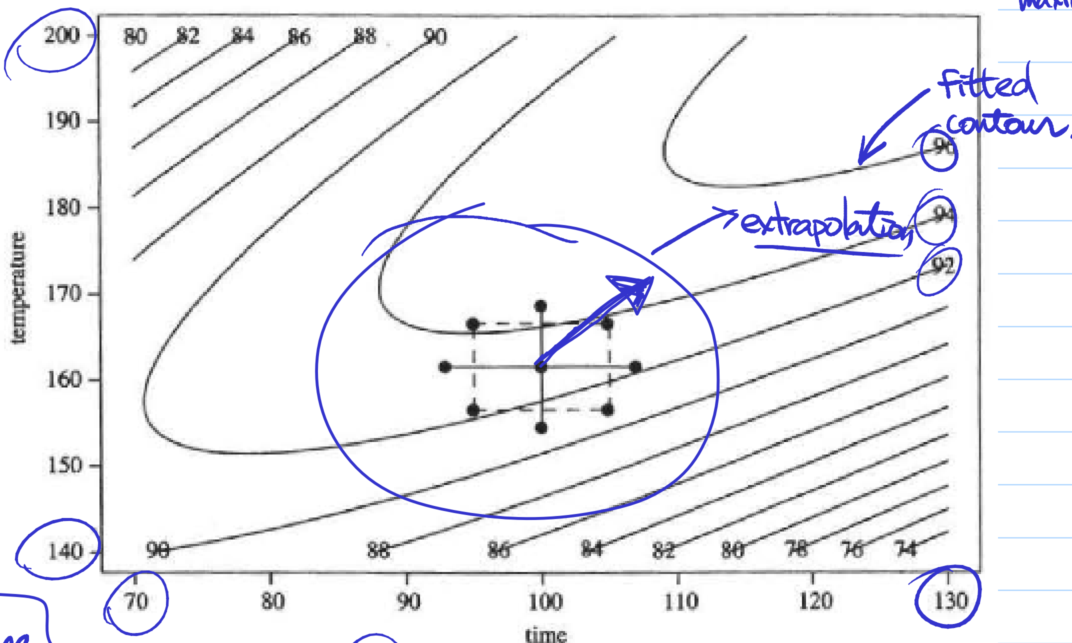
- The $\boxed{\text{contours}}$ of the fitted response surface are displayed in Figure 5. It suggests that moving in northeast direction would increase the yield.

c.f. direction is correct ← interpolation

but location of maximum is faulty ← extrapolation

Illustrated Second-Order Experiment

maximum



Q: If use different coding for effects, same conclusion?

c.f. → Figure 4 (LN p.3-20)

Figure 5: Fitted response surface

v **Reading**: textbook, 10.3.2