Steepest Ascent Search

- Suppose the fitted model is

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

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

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

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

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

and the **steepest descent** direction (for minimization) is

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

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 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.

Illustrated Initial First-Order Experiment

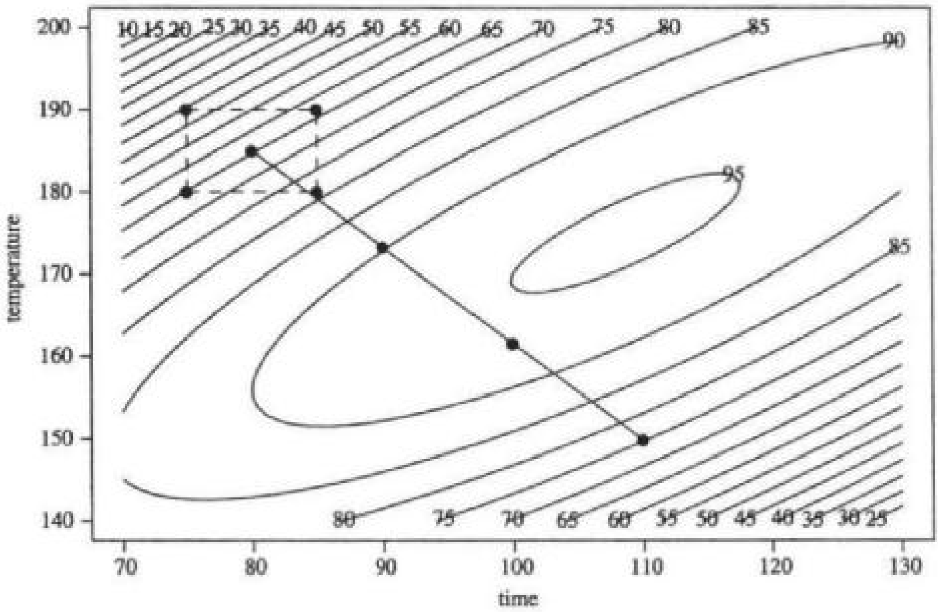

Figure 3: First-order experiment with steepest ascent

Illustrated Initial First-Order Experiment

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

	Factor		
Run	Time	Temperature	Yield
1	−1	−1	65.60
2	−1	1	45.59
3	1	−1	78.72
4	1	1	62.96
5	0	0	64.78
6	0	0	64.33
7	2	2(-1.173)	89.73
8	4	4(-1.173)	93.04
9	6	6(-1.173)	75.06

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

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

Illustrated Steepest Ascent Search

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

Illustrated Second-Order Experiment

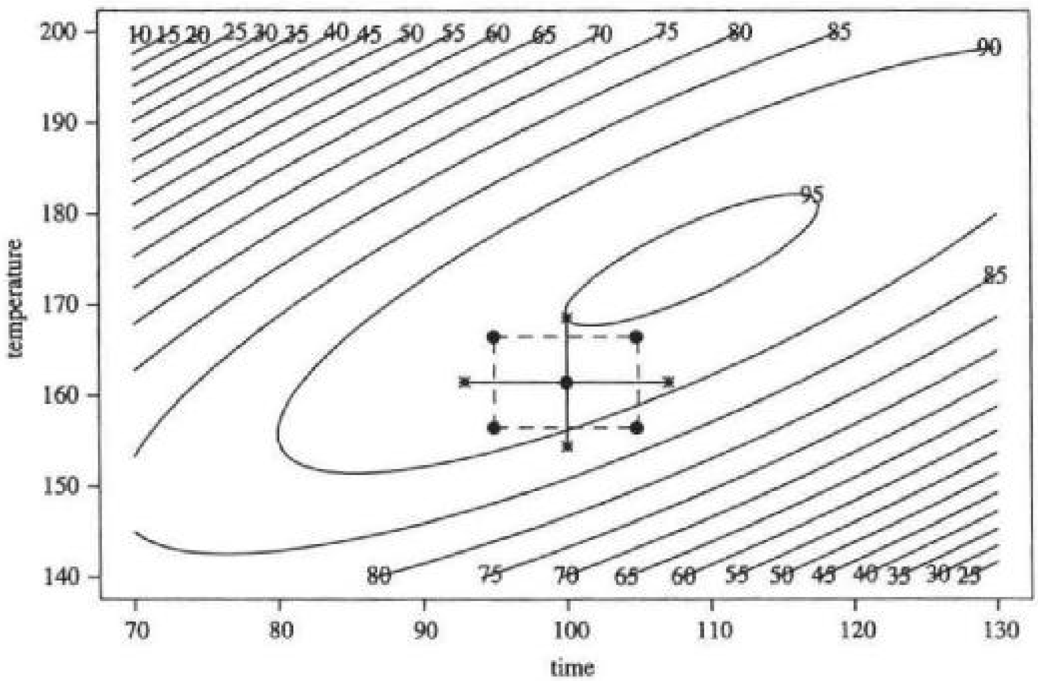

Figure 4: Second-order experiment

Illustrated Second-Order Experiment

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

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

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

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 second-order design
- 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 contours of the fitted response surface are displayed in Figure 5. It suggests that moving in northeast direction would increase the yield.

Illustrated Second-Order Experiment

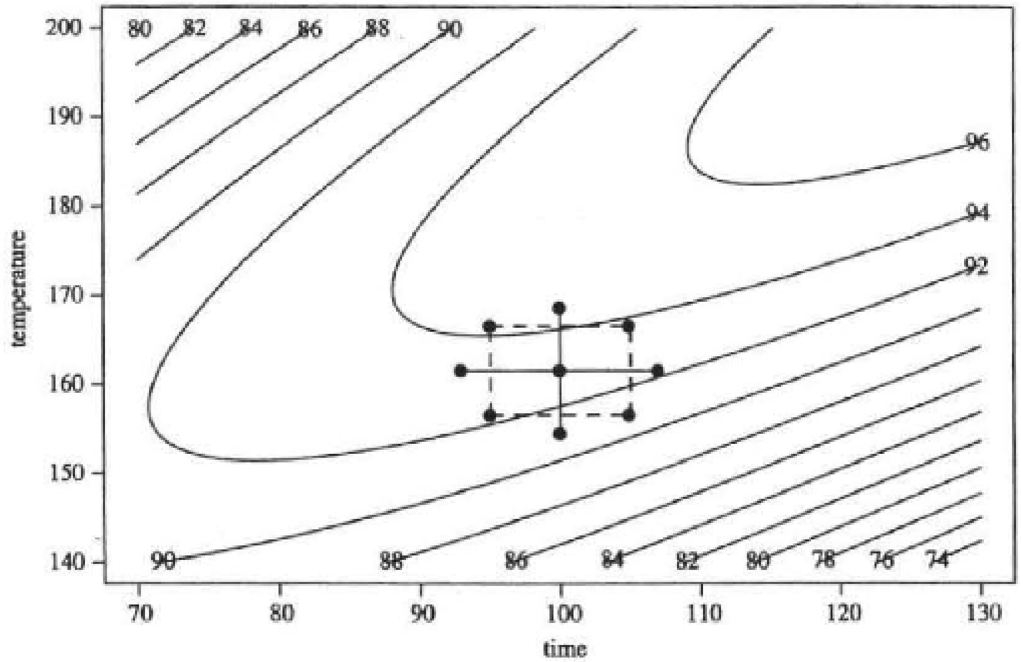

Figure 5: Fitted response surface

Reading: textbook, 10.3.2

Rectangular Grid Search

- Procedure
  - start with a first-order experiment with widely spaced factor levels
  - use the sign and magnitude of the main effect for each factor to narrow the search to a smaller range
  - perform a first- or second-order experiment over the smaller region of factor levels again
- Illustration

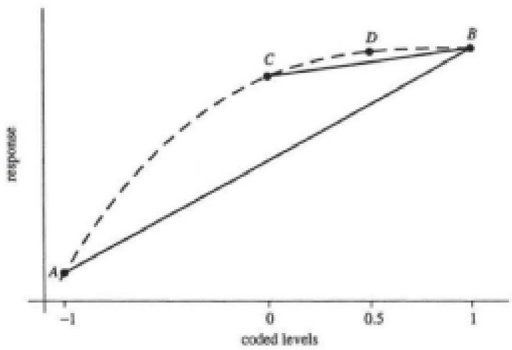

Figure 6: Search for the Peak of Unknown Response Curve (dashed curve): initial design over $[-1,1]$, second design over [0,1]

Reading: textbook, 10.3.3

Analysis of Second-Order Response Surface

- Fitted second-order model:

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i + \sum_{i<j}^{k} \hat{\beta}_{ij} x_i x_j + \sum_{i=1}^{k} \hat{\beta}_{ii} x_i^2,$$

- Matrix form

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}^T \mathbf{b} + \mathbf{x}^T \mathbf{B} \mathbf{x}, \qquad (3)$$

where $\mathbf{x}^T = (x_1, \ldots, x_k)$, $\mathbf{b}^T = (\hat{\beta}_1, \ldots \hat{\beta}_k)$, and $\mathbf{B}$ is the $k \times k$ symmetric matrix

$$\mathbf{B} = \begin{bmatrix} \hat{\beta}_{11} & \frac{1}{2}\hat{\beta}_{12} & \cdots & \frac{1}{2}\hat{\beta}_{1k} \\ \frac{1}{2}\hat{\beta}_{12} & \hat{\beta}_{22} & \cdots & \frac{1}{2}\hat{\beta}_{2k} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{1}{2}\hat{\beta}_{1k} & \frac{1}{2}\hat{\beta}_{2k} & \cdots & \hat{\beta}_{kk} \end{bmatrix}.$$

Analysis of Second-Order Response Surface

- Differentiating $\hat{y}$ in Eqn. (3) with respect to $\mathbf{x}$ and setting it to $\mathbf{0}$, we get

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0}, \qquad (4)$$

- The Eqn. (4) leads to the solution

$$\mathbf{x}_s = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b},$$

which is called the *stationary point* of the quadratic surface in Eqn. (3).

- To better understand the nature of the quadratic surface around the stationary point, use a new coordinate system
  - Let $\mathbf{P}$ be the $k \times k$ matrix whose columns are the standardized eigenvectors of $\mathbf{B}$.
  - Then

$$\mathbf{P}^T \mathbf{B} \mathbf{P} = \Lambda,$$

where $\Lambda = diag(\lambda_1, \ldots, \lambda_k)$ is a diagonal matrix and λ_i are the eigenvalues of $\mathbf{B}$ associated with the ith column of $\mathbf{P}$.

Analysis of Second-Order Response Surface

- *Translating* the model in Eqn. (3) to a new center, the stationary point, i.e.,

$$\mathbf{z} = \mathbf{x} - \mathbf{x}_s,$$

and *rotating* to new axes associated with the eigenvectors, i.e.,

$$\mathbf{v} = \mathbf{P}^T \mathbf{z} \quad (\Rightarrow \mathbf{z} = \mathbf{P}\mathbf{P}^T \mathbf{z} = \mathbf{P}\mathbf{v}).$$

- Under the new coordinate system, we have

$$\begin{aligned} \hat{y} &= \hat{\beta}_0 + (\mathbf{z}+\mathbf{x}_s)^T \mathbf{b} + (\mathbf{z}+\mathbf{x}_s)^T \mathbf{B}(\mathbf{z}+\mathbf{x}_s) \\ &= (\hat{\beta}_0 + \mathbf{x}_s{}^T \mathbf{b} + \mathbf{x}_s{}^T \mathbf{B}\mathbf{x}_s) + \mathbf{z}^T \mathbf{B}\mathbf{z} + \mathbf{z}^T \mathbf{b} + 2\mathbf{z}^T \mathbf{B}\mathbf{x}_s \\ &= \hat{y}_s + \mathbf{z}^T \mathbf{B}\mathbf{z} \\ &= \hat{y}_s + \mathbf{v}^T \mathbf{P}^T \mathbf{B}\mathbf{P}\mathbf{v} = \hat{y}_s + \mathbf{v}^T \Lambda \mathbf{v} = \hat{y}_s + \sum_{i=1}^{k} \lambda_i v_i^2, \end{aligned}$$

where $\hat{y}_s$ is the fitted response at $\mathbf{x}_s$.

Analysis of Second-Order Response Surface

- *Canonical analysis* of a second-order surface is based on
  - eigenvalues of **B**: $\lambda_1, \ldots, \lambda_k$
  - *canonical variables*: $v_1, \ldots, v_k$
- Calssification of different systems
  1. the λ_i's are of the same sign $\Rightarrow$ *elliptic system*
     - when the signs are negative, the stationary point is a point of *maximum* response
     - when the signs are positive, the stationary point is a point of *minimum* response
  2. the λ_i's are of mixed signs $\Rightarrow$ *hyperbolic system*
     - the stationary point is a *saddle* point
  3. one (or some) of the λ_i's is very close to 0 relative to the others $\Rightarrow$ *ridge system*

Analysis of Second-Order Response Surface

- Ridge system
  - stationary point inside the exp'tal region ⇒ *stationary ridge system*
    - ∗ line maximum ⇒ considerable *flexibility* in locating optimum operating conditions along a whole line (or plane)
  - stationary point far from the exp'tal region ⇒ *rising (falling) ridge system*
    - ∗ it suggests that movement outside the current region for additional experimentation is warranted

Analysis of Second-Order Response Surface

- Illustration

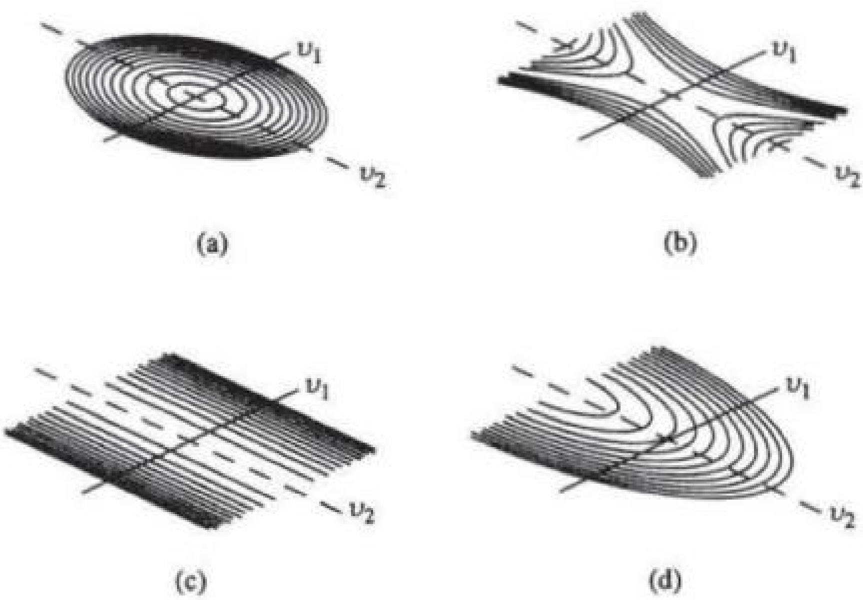

Figure 7: Classification of Second-Order Responses Surfaces: (a) elliptic, (b) hyperbolic, (c) stationary ridge, (d) rising ridge

v **Reading**: textbook, 10.4