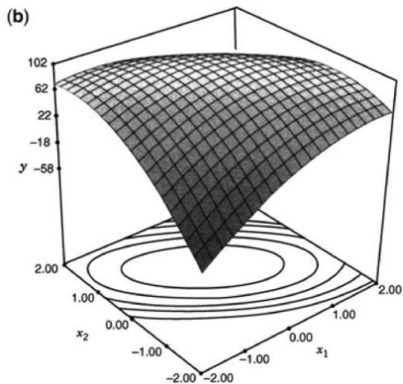
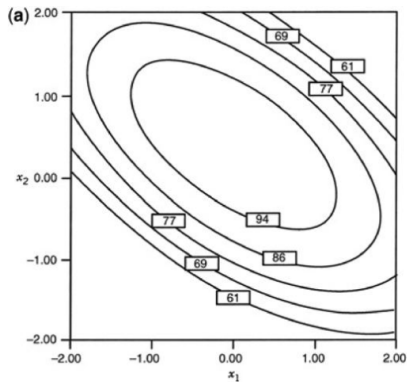


Response Surface Methodology: Optimizing Second-Order Models

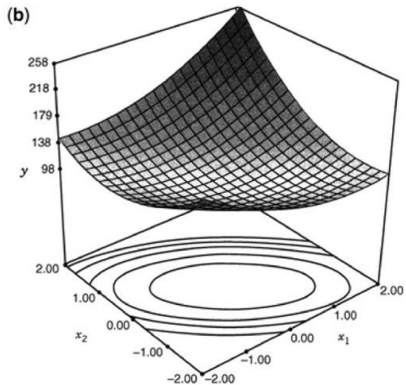
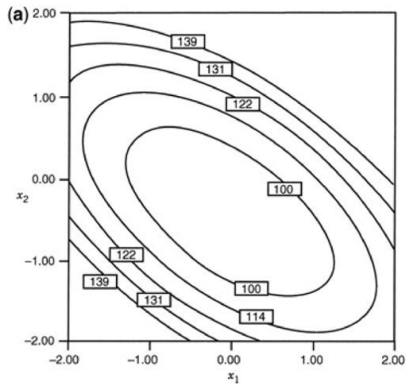
BIOE 498/598 PJ

Spring 2021

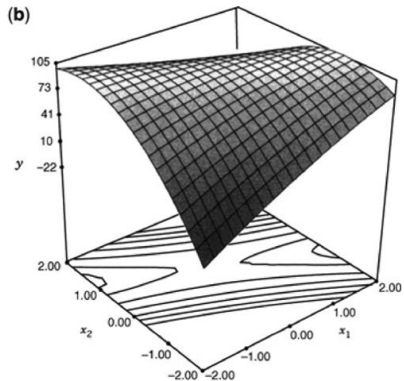
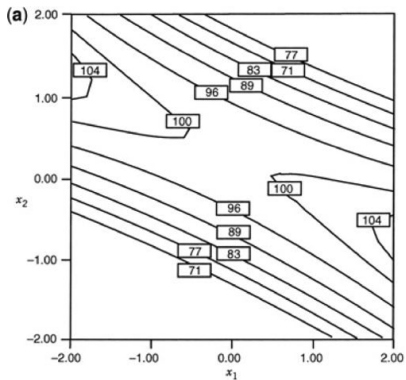
Second-order response surfaces: Maximum



Second-order response surfaces: Minimum



Second-order response surfaces: Saddle Point



Finding the response stationary point

The general second-order linear model is

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{j=1}^k \sum_{i=1}^{j-1} \beta_{ij} x_i x_j.$$

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We can rewrite this using matrix notation:

$$y = b_0 + \mathbf{x}^T \mathbf{b} + \mathbf{x}^T \mathbf{B} \mathbf{x}.$$

$$b_0 = \beta_0, \quad \mathbf{b} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_k \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} \beta_{11} & \beta_{12}/2 & \cdots & \beta_{1k}/2 \\ & \beta_{22} & \cdots & \beta_{2k}/2 \\ & & \ddots & \vdots \\ \text{sym} & & & \beta_{kk} \end{pmatrix}$$

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$$y = 3 - 0.3x_1 + x_2 + 1.2x_1^2 - 0.4x_1x_2$$

$$b_0 = 3, \quad \mathbf{b} = \begin{pmatrix} -0.3 \\ 1 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 1.2 & -0.2 \\ -0.2 & 0 \end{pmatrix}$$

Where is the stationary point?

The argmin, argmax, or inflection point of a saddle is called the **stationary point** (\mathbf{x}_s).

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Solving for where the derivative equals zero:

$$\mathbf{b} + 2\mathbf{B}\mathbf{x}_s = \mathbf{0} \Rightarrow \mathbf{x}_s = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

What is the response at the stationary point?

$$\begin{aligned}y_s &= b_0 + \mathbf{x}_s^\top \mathbf{b} + \mathbf{x}_s^\top \mathbf{B} \mathbf{x}_s \\&= b_0 + \mathbf{x}_s^\top \mathbf{b} + \left(-\frac{1}{2} \mathbf{b}^\top \mathbf{B}^{-1} \right) \mathbf{B} \mathbf{x}_s \\&= b_0 + \frac{1}{2} \mathbf{x}_s^\top \mathbf{b}\end{aligned}$$

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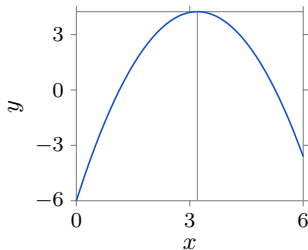
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Imagine a downward facing parabola

$$y = 3 + 0.4x - (x - 3)^2.$$

The argmax is $x_s = 3$ with response

$$\begin{aligned}y_s &= 3 + 0.4(3) - (3 - 3)^2 \\&= 3 + 1.2 - 0^2.\end{aligned}$$



Chemical Process Example (Myers 2016)

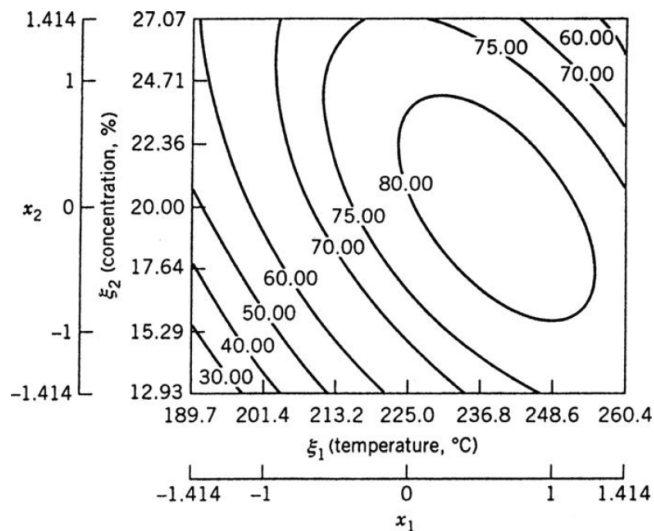
Observation	A		B		
	Temperature (°C) ξ_1	Conc. (%) ξ_2	x_1	x_2	y
1	200	15	-1	-1	43
2	250	15	1	-1	78
3	200	25	-1	1	69
4	250	25	1	1	73
5	189.65	20	-1.414	0	48
6	260.35	20	1.414	0	76
7	225	12.93	0	-1.414	65
8	225	27.07	0	1.414	74
9	225	20	0	0	76
10	225	20	0	0	79
11	225	20	0	0	83
12	225	20	0	0	81

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$$b_0 = 79.75, \quad \mathbf{b} = \begin{pmatrix} 10.12 \\ 4.22 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} -8.50 & -3.875 \\ -3.875 & -5.25 \end{pmatrix}$$

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$$\begin{aligned} \mathbf{x}_s &= -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b} \\ &= -\frac{1}{2} \begin{pmatrix} -0.1773 & 0.1309 \\ 0.1309 & -0.2871 \end{pmatrix} \begin{pmatrix} 10.12 \\ 4.22 \end{pmatrix} \\ &= \begin{pmatrix} 0.6264 \\ -0.0604 \end{pmatrix} \end{aligned}$$

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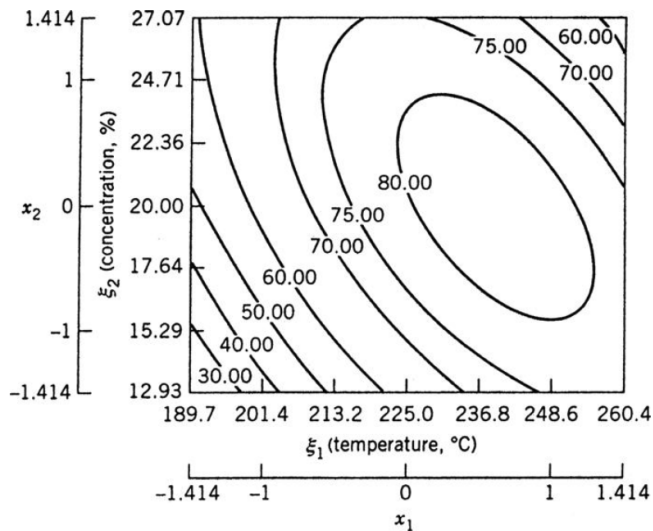
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$$\text{Temperature} = 225 + 25x_{1,s} = 225 + 25(0.6264) = 240^\circ\text{C}$$

$$\text{Concentration} = 20 + 5x_{2,s} = 20 + 5(-0.0604) = 19.7\%$$

Visual confirmation of stationary point



Temperature = 240°C

Concentration = 19.7%

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- ▶ In the previous example, $\lambda_1 = -11.0769$ and $\lambda_2 = -2.6731$, so \mathbf{x}_s is an argmax.

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or, more simply,

$$y = y_s + \sum_{i=1}^k \lambda_i w_i^2$$

*Canonical analysis

$$\mathbf{w} = \mathbf{V}^T(\mathbf{x} - \mathbf{x}_s)$$

$$y = y_s + \sum_{i=1}^k \lambda_i w_i^2$$

