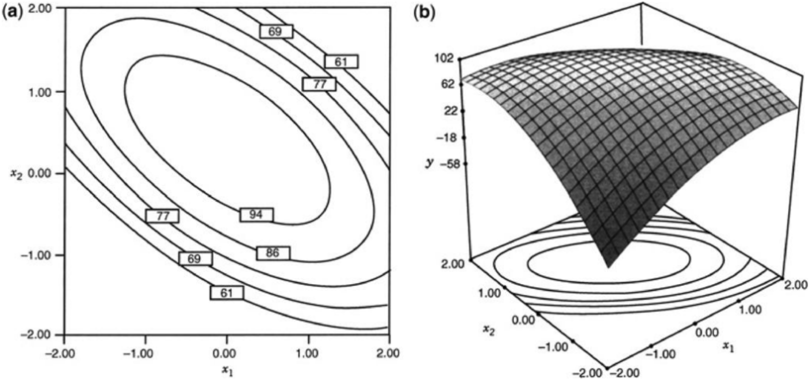
Response Surface Methodology: Optimizing Second-Order Models

BIOE 498/598 PJ

Spring 2022

Second-order response surfaces: Maximum



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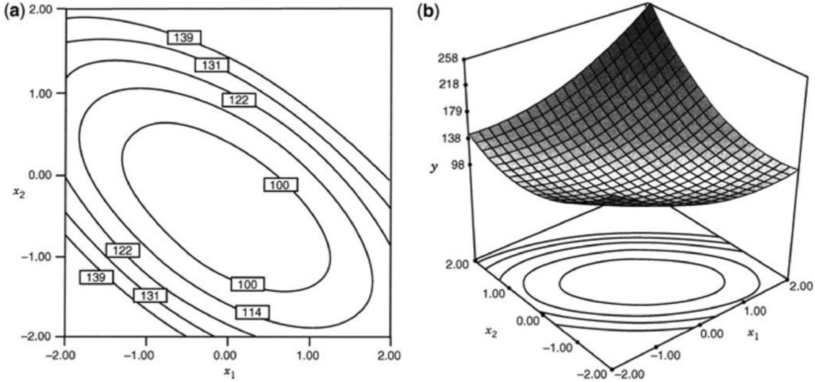
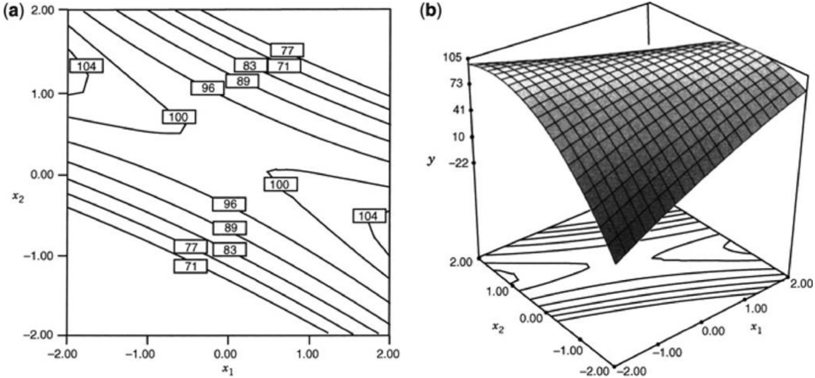


Second-order response surfaces: Saddle Point



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:

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

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

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

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

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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{}^{\mathsf{T}}\mathbf{b} + \mathbf{x}_s{}^{\mathsf{T}}\mathbf{B}\mathbf{x}_s \\
&= b_0 + \mathbf{x}_s{}^{\mathsf{T}}\mathbf{b} + \left(-\frac{1}{2}\mathbf{b}^{\mathsf{T}}\mathbf{B}^{-1}\right)\mathbf{B}\mathbf{x}_s \\
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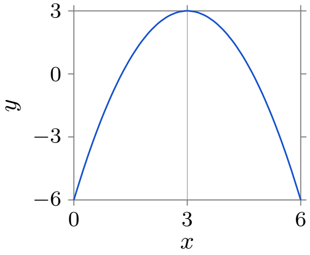
Imagine a downward facing parabola

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

The argmax is $x_s = 3$ with response

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



Chemical Process Example (Myers 2016)

	A		B		
Observation	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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$$y = 79.75 + 10.18x_1 + 4.22x_2 - 8.50x_1^2 - 5.25x_2^2 - 7.75x_1x_2$$

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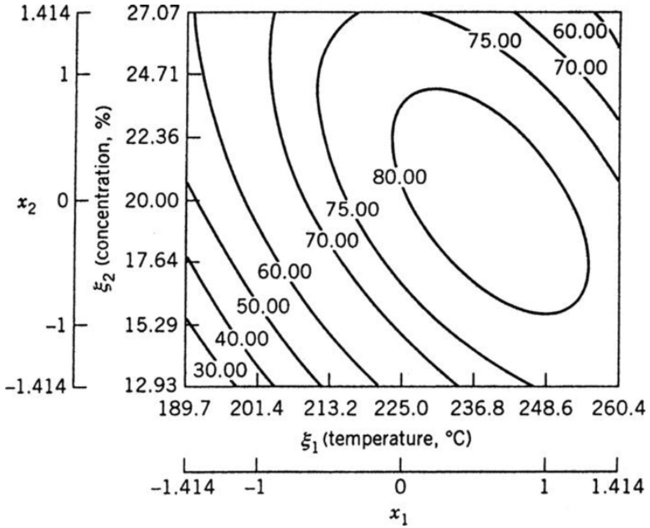

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$$b_0 = 79.75, \quad \mathbf{b} = \begin{pmatrix} 10.12 \\ 4.22 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} -8.50 & -3.875 \\ -3.875 & -5.25 \end{pmatrix}$$

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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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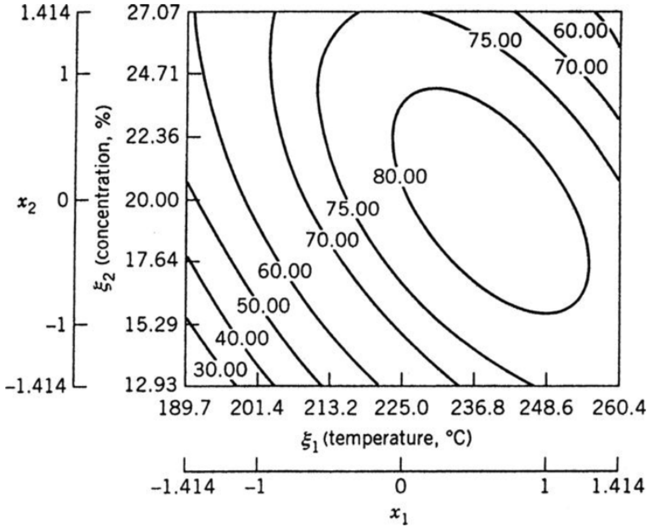
Temperature $= 225 + 25x_{1,s} = 225 + 25(0.6264) = 240°$C

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

Visual confirmation of stationary point



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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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Let $\mathbf{V}$ be a matrix with columns equal to the eigenvectors of $\mathbf{B}$, and let

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The response anywhere can be defined in terms of the **canonical vector** $\mathbf{w}$ an a diagonal matrix of eigenvalues $\mathbf{\Lambda}$,

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or, more simply,

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

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