

EXAMPLE 6.15

ORIGIN := 1

$$x_1 := \begin{pmatrix} 0.0563 \\ 0.0563 \\ 0.1643 \\ 0.2520 \\ 0.2666 \\ 0.2666 \\ 0.3661 \\ 0.4732 \\ 0.4732 \\ 0.5740 \\ 0.5740 \\ 0.6690 \\ 0.7587 \\ 0.8435 \\ 0.9238 \end{pmatrix} \quad \Delta H_{\text{mix}} := \begin{pmatrix} 150.8 \\ 147.4 \\ 375.2 \\ 500.1 \\ 519.0 \\ 520.2 \\ 609.6 \\ 630.9 \\ 644.3 \\ 618.7 \\ 618.1 \\ 567.7 \\ 478.3 \\ 351.5 \\ 199.7 \end{pmatrix}$$

i := 1 .. 15

$$x_{2,i} := 1 - x_{1,i}$$

$$y_i := \frac{\Delta H_{\text{mix},i}}{x_{1,i} \cdot x_{2,i}} \quad z_i := x_{1,i} - x_{2,i}$$

$$\begin{bmatrix} 15 & \sum_i z_i & \sum_i (z_i)^2 & \sum_i (z_i)^3 \\ \sum_i z_i & \sum_i (z_i)^2 & \sum_i (z_i)^3 & \sum_i (z_i)^4 \\ \sum_i (z_i)^2 & \sum_i (z_i)^3 & \sum_i (z_i)^4 & \sum_i (z_i)^5 \\ \sum_i (z_i)^3 & \sum_i (z_i)^4 & \sum_i (z_i)^5 & \sum_i (z_i)^6 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \sum_i y_i \\ \sum_i (z_i \cdot y_i) \\ \sum_i [(z_i)^2 \cdot y_i] \\ \sum_i [(z_i)^3 \cdot y_i] \end{bmatrix} = \begin{pmatrix} 2.546 \times 10^3 \\ -125.091 \\ 361.22 \\ 197.836 \end{pmatrix}$$

Alternative Approach - 1

$$F(z) := \begin{pmatrix} 1 \\ z \\ z^2 \\ z^3 \end{pmatrix}$$

$$C := \text{linfit}(z, y, F) = \begin{pmatrix} 2.546 \times 10^3 \\ -125.091 \\ 361.22 \\ 197.836 \end{pmatrix}$$

$$g(z) := F(z) \cdot C$$

$$\text{corr}(\vec{g(z)}, y) = 0.979$$

Alternative Approach - 2

$$G(A_1, A_2, A_3, A_4) := \sum_{i=1}^{15} \left[y_i - \left[A_1 + A_2 \cdot z_i + A_3 \cdot (z_i)^2 + A_4 \cdot (z_i)^3 \right] \right]^2$$

Initial guess values

$$A_1 := 2500 \quad A_2 := -100 \quad A_3 := 300 \quad A_4 := 200$$

Given

$$\frac{d}{dA_1} G(A_1, A_2, A_3, A_4) = 0$$

$$\frac{d}{dA_2} G(A_1, A_2, A_3, A_4) = 0$$

$$\frac{d}{dA_3} G(A_1, A_2, A_3, A_4) = 0$$

$$\frac{d}{dA_4}G(A_1, A_2, A_3, A_4) = 0$$

$$\text{Find}(A_1, A_2, A_3, A_4) = \begin{pmatrix} 2.546 \times 10^3 \\ -125.091 \\ 361.22 \\ 197.836 \end{pmatrix}$$