

Multivariate Regression models



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Multiple Linear Regression model

x_1 Age	x_2 Income (hundred thousand dollar)	y Balance (thousand dollar)
32	0.550798	5.651202
22	0.708148	7.321263
45	0.290905	5.167304
78	0.510828	5.609367
54	0.892947	9.406379
39	0.896293	9.379439
42	0.125585	2.734997
51	0.207243	4.876649
21	0.051467	3.584138
19	0.44081	5.437239

$$(x_1, x_2) \rightarrow y$$

Multiple Linear Regression model

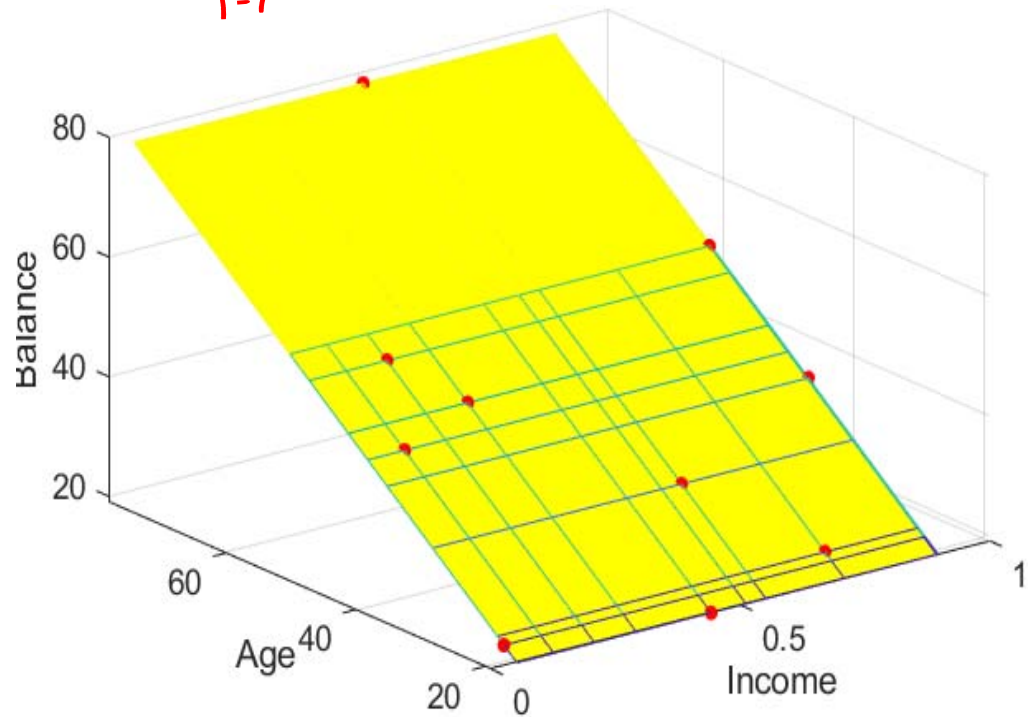
$$X \rightarrow y$$

$$f(x) = \beta_1 x_1 + \beta_2 x_2 + \beta_0$$

$$\sum_{i=1}^n (y_i - f(x_i))^2$$

x_1 Age	x_2 Income (hundred thousand dollar)	y Balance (thousand dollar)
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19	0.44081	5.437239

x_1
 x_2



For given Training Set $T = \{ (x_{11}, x_{12}, y_1), (x_{21}, x_{22}, y_2), \dots, (x_{n1}, x_{n2}, y_n) \}$, we need to solve

$$\text{Min } J(\beta_5, \beta_4, \beta_3, \beta_2, \beta_1, \beta_0) = \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i}))^2 \dots (1)$$

$$u = \begin{bmatrix} \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix}$$

$A =$

$$\begin{bmatrix} x_{11} & x_{12} & 1 \\ x_{21} & x_{22} & 1 \\ \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & 1 \end{bmatrix}$$

$$\begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_0 \end{bmatrix}$$

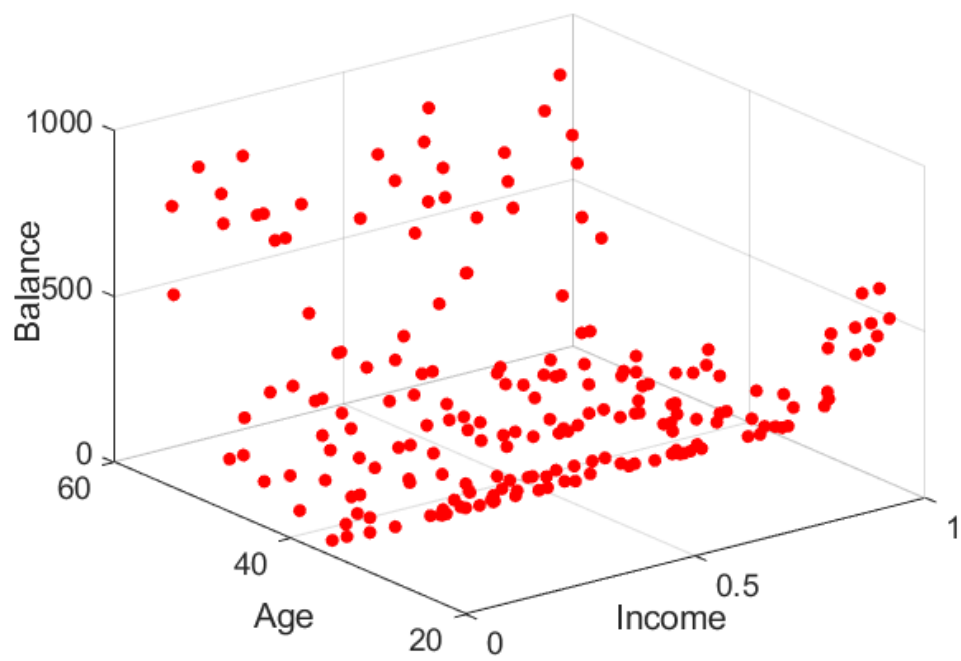
$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{aligned} &\beta_1 x_{11} + \beta_2 x_{12} + \beta_0 \\ &\beta_1 x_{21} + \beta_2 x_{22} + \beta_0 \\ &\vdots \\ &\beta_1 x_{n1} + \beta_2 x_{n2} + \beta_0 \end{aligned}$$

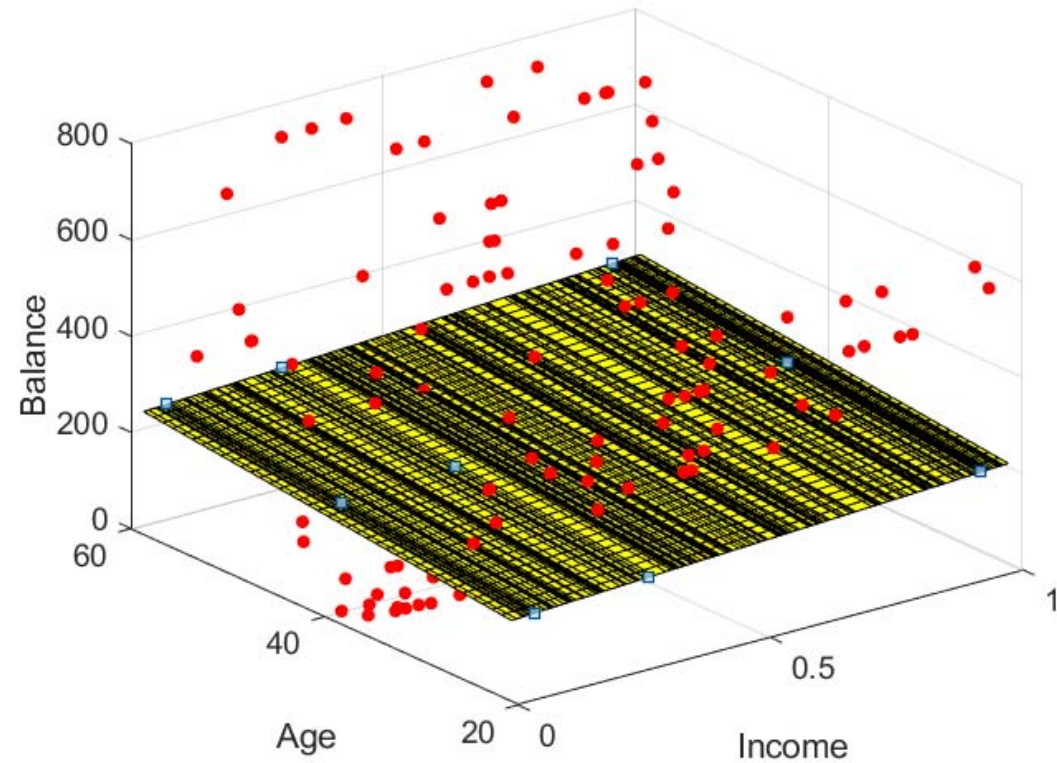
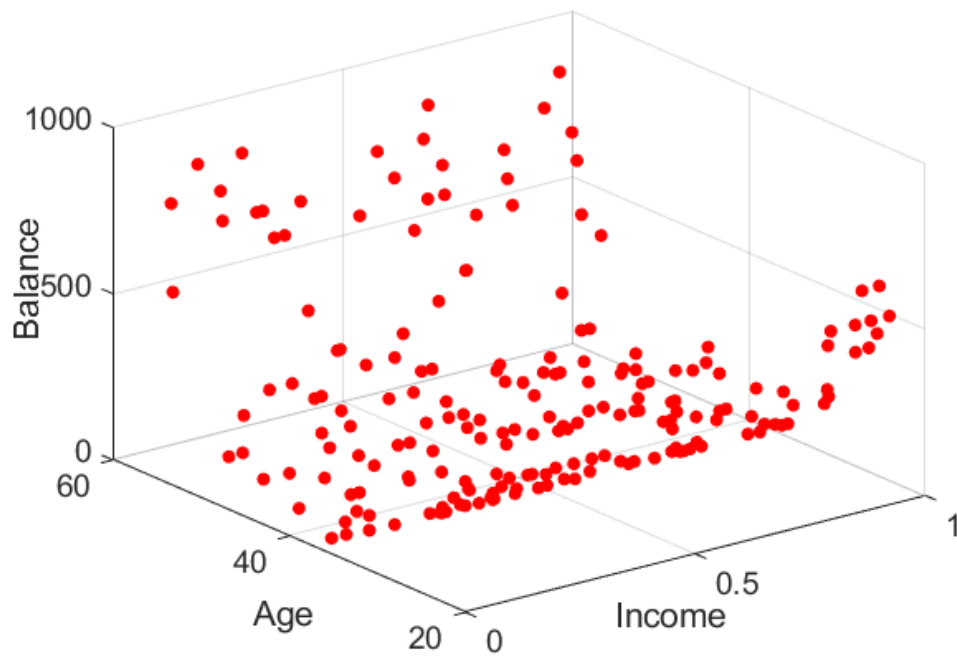
The Least Square problem reduces to

$$\text{Min}_{(u)} J(u) = (Y - Au)^T (Y - Au)$$

$$u = \begin{bmatrix} \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} = (A^T A)^{-1} A^T Y$$

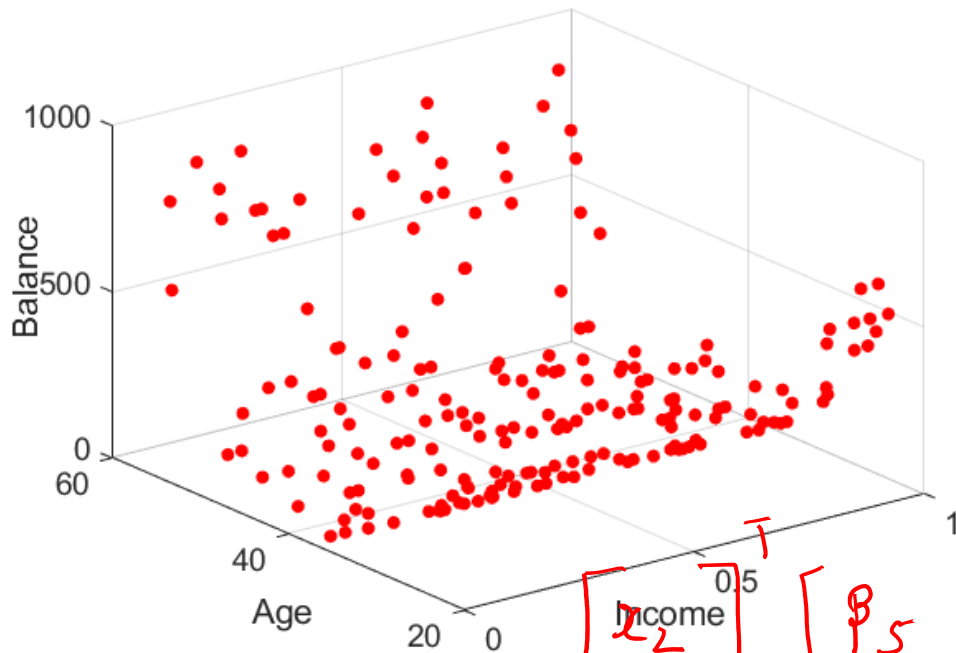


Quadratic Regression model with two variables



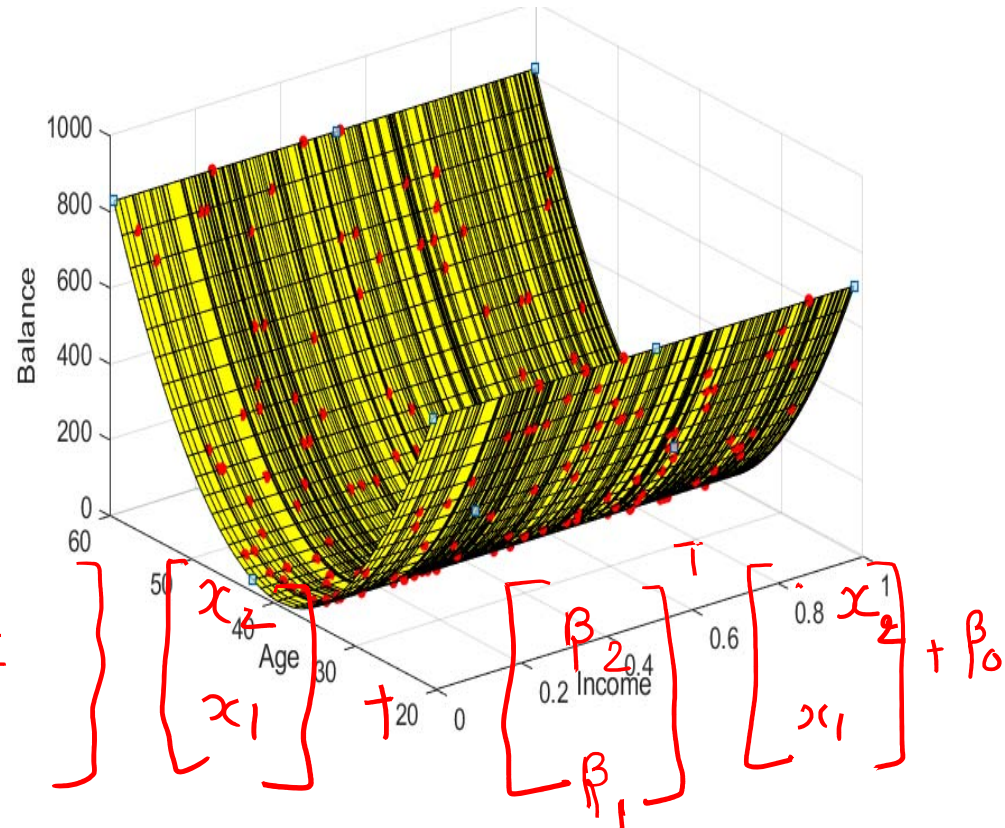
Quadratic Regression model with two variables

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 x_1^2 + \beta_5 x_2^2$$



$$\begin{bmatrix} x_2 \\ x_1 \end{bmatrix}^T \begin{bmatrix} \beta_5 \\ \beta_3 \end{bmatrix}$$

$$\frac{\beta_3}{2}$$



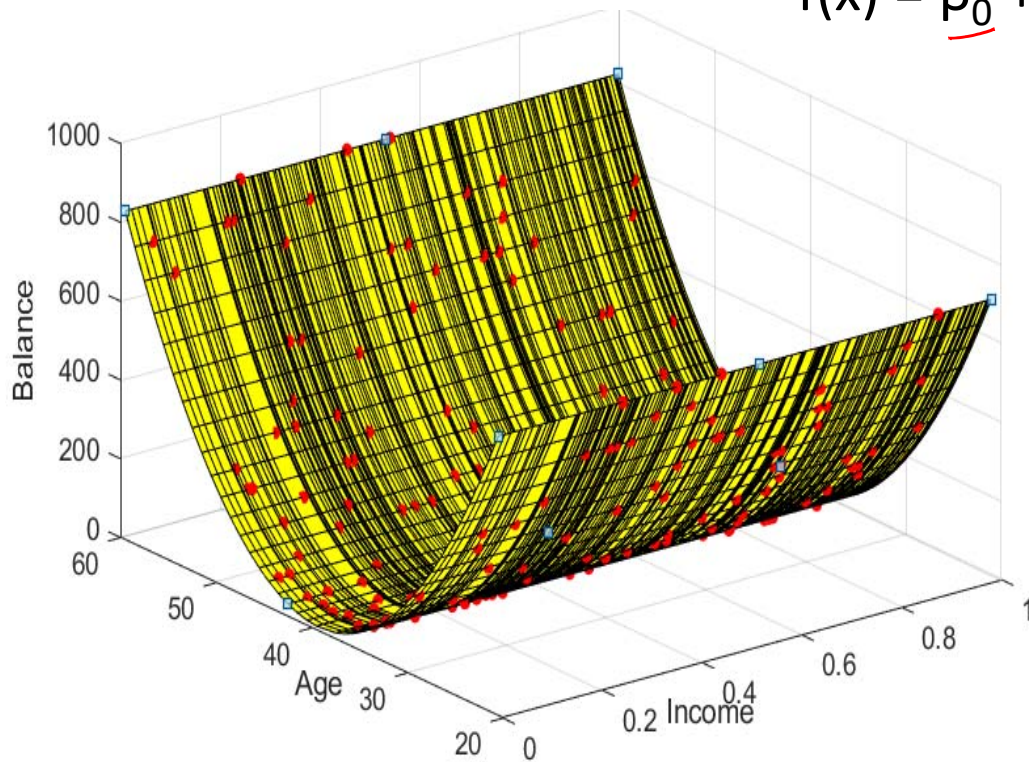
$$\begin{bmatrix} x_2 \\ x_1 \end{bmatrix}$$

$$\begin{bmatrix} \beta_2 \\ \beta_1 \end{bmatrix}^T \begin{bmatrix} x_2 \\ x_1 \end{bmatrix}$$

$$+ \beta_0$$

Quadratic Regression model with two variables

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 x_2^2 + \beta_5 x_1^2$$



$$\sum_{i=1}^n$$

For given Training Set $T = \{(\underbrace{x_{11}, x_{12}}_{x_1}, y_1), (\underbrace{x_{21}, x_{22}}_{x_2}, y_2), \dots, (\underbrace{x_{n1}, x_{n2}}_{x_n}, y_n)\}$, we need to solve

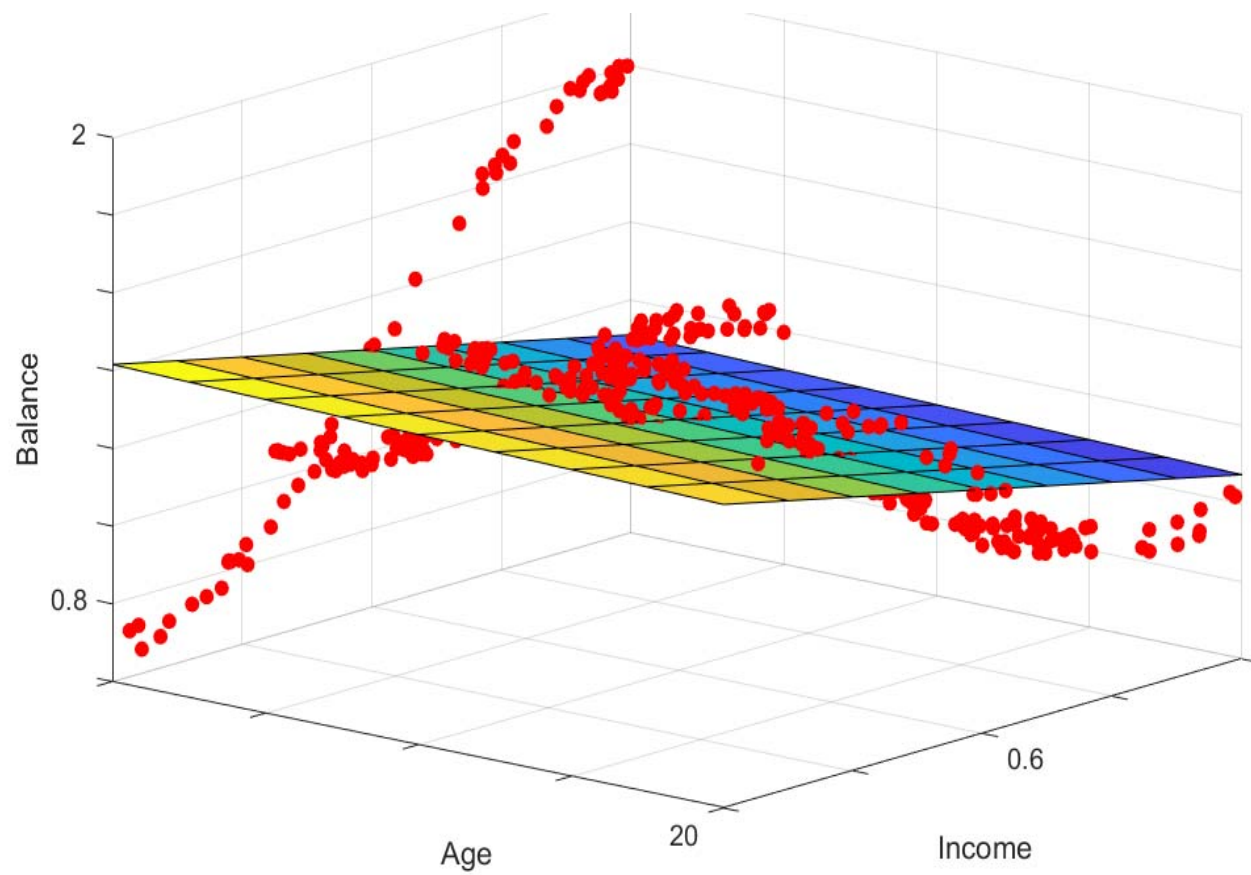
$$\text{Min } J(\beta_5, \beta_4, \beta_3, \beta_2, \beta_1, \beta_0) = \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i} x_{2i} + \beta_4 x_{2i}^2 + \beta_5 x_{1i}^2))^2 \quad \dots (1)$$

$$u = \begin{bmatrix} \beta_5 \\ \beta_4 \\ \beta_3 \\ \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} \quad A = \begin{bmatrix} x_{11}^2 & x_{21}^2 & x_{11} x_{21} & x_{21} & x_{11} & 1 \\ x_{21}^2 & x_{22}^2 & x_{21} x_{22} & x_{22} & x_{21} & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1}^2 & x_{n2}^2 & x_{n1} x_{n2} & x_{n2} & x_{n1} & 1 \end{bmatrix} \begin{matrix} \beta_5 \\ \beta_4 \end{matrix} \quad Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

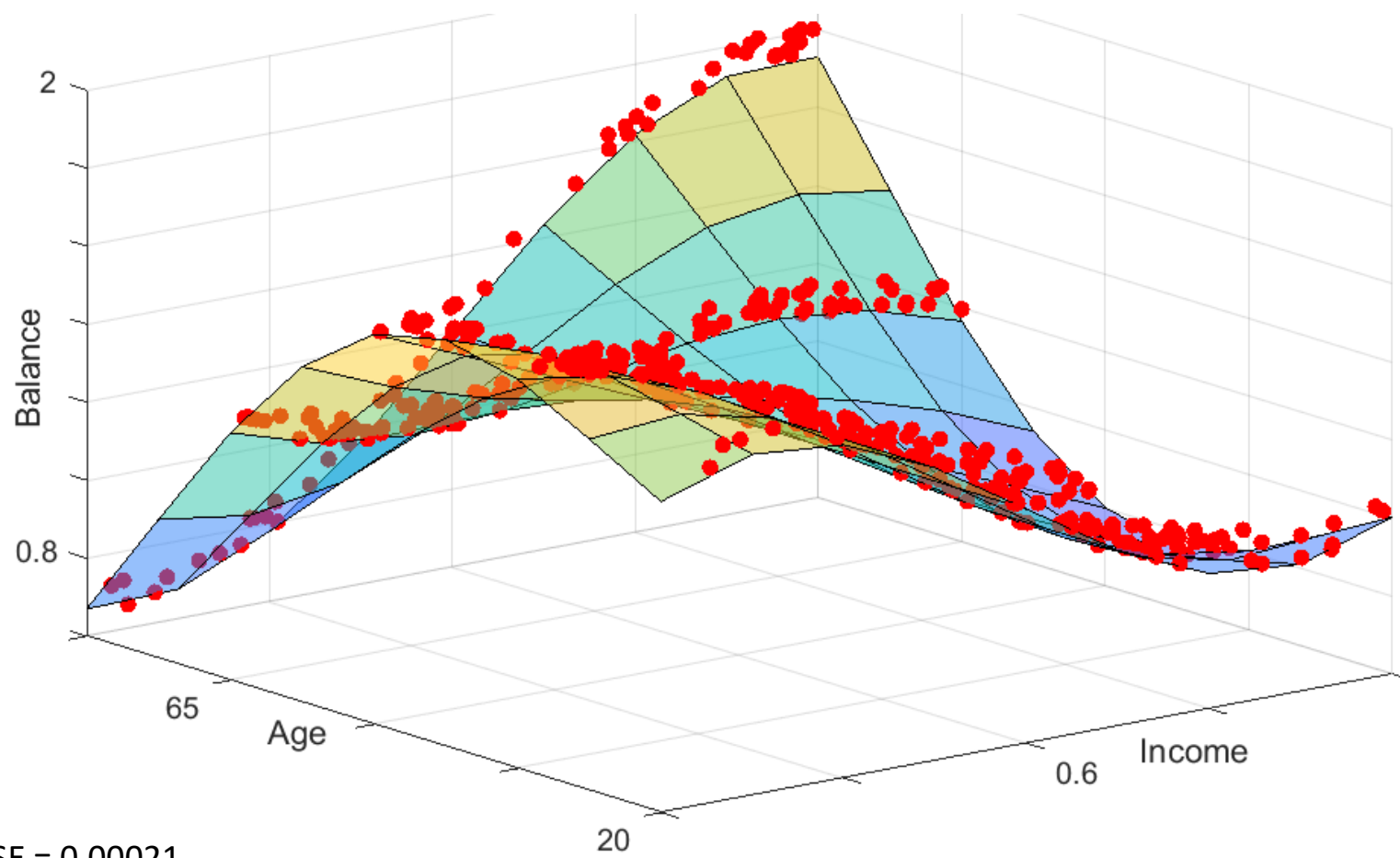
The Least Square problem reduces to

$$\text{Min}_{(u)} J(u) = \frac{1}{2} (Y - Au)^T (Y - Au)$$

$$u = \begin{bmatrix} \beta_5 \\ \beta_4 \\ \beta_3 \\ \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} = (A^T A)^{-1} A^T Y$$



Train RMSE = 0.4621



Train RMSE = 0.00021

$$\begin{array}{l}
 x_2^3 \rightarrow \phi_9(x) \\
 x_1^3 \rightarrow \phi_8(x) \\
 x_1 x_2^2 \rightarrow \phi_7(x) \\
 x_1^2 x_2 \\
 x_2^2 \\
 x_1^2 \\
 x_1 x_2 \\
 x_2 \\
 x_1 \\
 \textcircled{1} \rightarrow \phi_0(x)
 \end{array}$$

$$\phi(x) = \begin{bmatrix} \phi_9(x) \\ \phi_8(x) \\ \vdots \\ \phi_0(x) \end{bmatrix}$$

$$w^T \phi(x) = ?$$

$$w = \begin{bmatrix} \beta_9 \\ \beta_8 \\ \vdots \\ \beta_0 \end{bmatrix}$$

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\frac{(m+n)!}{m! n!}$$

$$x \in \mathbb{R}^2 \quad (\underline{x_1}, \underline{x_2})$$

$$\phi_0(x) = 1$$

$$\phi_1(x) = x_1$$

$$\phi_2(x) = x_2$$

$$\textcircled{w^T x}$$

$$w = \begin{bmatrix} \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ x_2 \\ 1 \end{bmatrix}$$

$$\min_{w \in \mathbb{R}^{10}} \frac{1}{n} \sum_{i=1}^n (y_i - \omega^T \phi(x_i))^2, \text{ where}$$

$$A = \begin{bmatrix} x_{12}^3 & x_{11}^3 & x_{11}x_{12}^2 & x_{11}^2x_{12} & \dots & 1 \\ x_{22}^3 & x_{21}^3 & x_{21}x_{22}^2 & x_{21}^2x_{22} & & 1 \\ - & - & - & - & & - \\ x_{n2}^3 & x_{n1}^3 & x_{n1}x_{n2}^2 & x_{n1}^2x_{n2} & \dots & 1 \end{bmatrix}$$

$$\phi(x_i) = \begin{bmatrix} \phi_9(x_i) \\ \phi_0(x_i) \end{bmatrix} = \begin{bmatrix} x_{2i}^3 \\ x_{1i}^3 \\ x_{1i}^2x_{2i} \\ \vdots \\ 1 \end{bmatrix}$$

$$A_4 = \begin{bmatrix} \beta_9 x_{12}^3 + \beta_8 x_{11}^3 + \beta_7 x_{11}x_{12}^2 + \dots & \beta_0 \\ \beta_9 x_{22}^3 + \beta_8 x_{21}^3 + \beta_7 x_{21}x_{22}^2 + \dots & \beta_0 \\ \vdots & \vdots \end{bmatrix}$$

$$\Delta = \begin{bmatrix} \Phi_9(x_1), \Phi_8(x_1) & \dots & \Phi_0(x_1) \\ \Phi_9(x_2) & \Phi_8(x_2) & & \Phi_0(x_2) \\ & & & \Phi_0(x_n) \end{bmatrix}$$

$$y = \bar{w} = \begin{bmatrix} \beta_9 \\ \vdots \\ \beta_0 \end{bmatrix} = (\Delta^T \Delta)^{-1} \Delta^T y$$

Multiple Regression model working with k variables

x_1	x_2	x_3	--	x_k	y Balance (thousand dollar)
32	0.550798	283	--	2	5.651202
22	0.708148	483	-	3	7.321263
45	0.290905	514	-	4	5.167304
78	0.510828	681	-	3	5.609367
54	0.892947	357	-	2	9.406379
39	0.896293	569	-	4	9.379439
42	0.125585	259	-	2	2.734997
51	0.207243	512	-	2	4.876649
21	0.051467	266	-	5	3.584138
19	0.44081	491	-	3	5.437239

$$\bar{w} \in \mathbb{R}^{k+1}$$

$$w^T \phi(x)$$

Multiple Regression model working with k variables

$$\bar{w}^T \bar{x}$$

$$w^T x + \beta_0$$

$$W = \begin{bmatrix} \beta_k \\ \beta_{k-1} \\ \vdots \\ \beta_1 \\ \beta_0 \end{bmatrix}$$

$$\bar{x} = \begin{bmatrix} x_k \\ x_{k-1} \\ \vdots \\ x_1 \\ 1 \end{bmatrix}$$

Linear Function:-

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \dots + \beta_k x_k$$

$$w \in \mathbb{R}^k \quad b \in \mathbb{R}$$

$$w^T x + b$$

For given Training Set $T = \{(x_{11}, x_{12}, \dots, x_{1k}, y_1), (x_{21}, x_{22}, \dots, x_{2k}, y_2), \dots, (x_{n1}, x_{n2}, \dots, x_{nk}, y_n)\}$, we solve

$$\text{Min } J(\beta_k, \dots, \beta_4, \beta_3, \beta_2, \beta_1, \beta_0) = \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \dots + \beta_k x_{ik}))^2$$

$$u = \begin{bmatrix} \beta_k \\ \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} \quad A = \begin{bmatrix} x_{11} & x_{21} & \dots & x_{1k} & 1 \\ x_{21} & x_{22} & \dots & x_{2k} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nk} & 1 \end{bmatrix}$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

The Least Square problem reduces to

$$\text{Min}_{(u)} J(u) = (Y - Au)^T (Y - Au)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$u = \begin{bmatrix} \beta_k \\ \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} = (A^T A)^{-1} A^T Y$$

https://colab.research.google.com/drive/1APfTBXi3U_1ADX1PmLkJ8DyhVCQBegtE?usp=sharing

$$\begin{aligned}
\beta_0 &\leftarrow \phi_0(x) = 1 \\
\beta_1 &\leftarrow \phi_1(x) = x_1 \\
&\phi_2(x) = x_3 \\
&\vdots \\
&\phi_k(x) = x_k \\
&\phi_{k+1}(x) = x_1 x_2 \\
&\phi_{k+2}(x) = x_2 x_3 \\
&\vdots \\
\beta_m &\leftarrow \phi_m(x) = x_k^2
\end{aligned}$$

$$\begin{aligned}
m &= \frac{(k+1)(k+2)}{2} \\
&\rightarrow x \in \mathbb{R}^n \quad x = \frac{(k+2)!}{k! 2!} \\
&= \sum_{i=0}^m \beta_i \phi_i(x) = w^T \Phi(x)
\end{aligned}$$

$$\Rightarrow w = \begin{bmatrix} \beta_m \\ \beta_{m-1} \\ \vdots \\ \beta_1 \\ \beta_0 \end{bmatrix}$$

$$\Phi(x) = \begin{bmatrix} \phi_m(x) \\ \phi_{m-1}(x) \\ \vdots \\ \phi_1(x) \\ \phi_0 \end{bmatrix}$$

$$\min_w \sum_{i=1}^N (y_i - w^T \Phi(x_i))^2$$

$$w = (A^T A)^{-1} A^T y$$

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_0 \end{bmatrix}$$

$$\min_{\beta_0, \beta_1, \beta_2} \left(\sum_{i=1}^N (y_i - \{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}\})^2 \right)$$

$$(y - Au) = \begin{bmatrix} y_1 - \beta_2 x_{12} \\ y_2 - \beta_2 x_{22} \\ \vdots \\ y_n - \beta_2 x_{n2} \end{bmatrix}$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad A = \begin{bmatrix} x_{11} & x_{12} & 1 \\ x_{21} & x_{22} & 1 \\ \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & 1 \end{bmatrix} \quad u = \begin{bmatrix} \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix}$$

$$y_i -$$

$$(y - Au) = \begin{bmatrix} y_1 - \beta_2 x_{11} - \beta_1 x_{12} - \beta_0 \\ \vdots \end{bmatrix}$$

$$\min_u (y - Au)^T (y - Au) =$$

$$A^T (y - Au) = 0$$

$$\Rightarrow u = (A^T A)^{-1} A^T y$$

$$f(x) = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{1i} x_{2i} + \beta_4 x_{1i}^2 + \beta_5 x_{2i}^2$$

$\phi_1(x)$ $\phi_2(x)$ $\phi_3(x)$ $\phi_4(x)$ $\phi_5(x)$
 \downarrow \downarrow \downarrow \downarrow \downarrow
 x_{1i}^2 x_{2i}^2 $x_{1i} x_{2i}$ x_{1i} x_{2i}

$$\begin{bmatrix} x_{11}^2 & x_{21}^2 & x_{11} x_{21} & x_{11} & x_{21} & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1}^2 & x_{n2}^2 & x_{n1} x_{n2} & x_{n1} & x_{n2} & 1 \end{bmatrix}$$

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 x_1^2 + \beta_5 x_2^2 + \beta_6 x_1 x_2^2 + \beta_7 x_1^2 x_2 + \beta_8 x_1^3 + \beta_9 x_2^3$$

$$\phi_0(x) = 1 = W^T \phi(x)$$

$$\phi(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \vdots \\ \phi_q(x) \end{bmatrix}$$

$$\phi_1(x) = x_1$$

$$\phi_2(x) = x_2$$

\vdots

$$\phi_q(x) = x_2^3$$

$$W = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_q \end{bmatrix}$$

$$A = \begin{bmatrix} \cancel{1} & \phi_0(x_1) & \phi_1(x_1) & \dots & \phi_q(x_1) \\ \phi_0(x_2) & - & - & - & - \\ \vdots & & & & \\ \phi_0(x_n) & \phi_1(x_n) & & & \phi_q(x_n) \end{bmatrix}$$

$$f(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \beta_{k+1} x_1 x_2 + \beta_{k+2} x_2 x_3 + \dots$$

(k-dim.
m-order)

$$+ \beta_m x_k^m$$

where

$$M = \frac{k! m!}{k!}$$

$$M = \frac{(k+m)!}{k! m!}$$

$$M = \frac{(k+m)!}{k! m!}$$

$$\omega = \begin{bmatrix} \beta_m \\ \beta_{m-1} \\ \vdots \\ \beta_1 \\ \beta_0 \end{bmatrix}$$

\Rightarrow Now,

$$\Rightarrow \text{Here, } \Phi_0(x) = 1$$

$$\Phi_1(x) = x_1$$

$$\Phi_2(x) = x_2$$

\vdots

$$\Phi_m(x) = x_k^m$$

$$f(x) = \omega^T \Phi(x)$$

$$\Phi(x) = \begin{bmatrix} \Phi_m(x) \\ \Phi_{m-1}(x) \\ \vdots \\ \Phi_0(x) \end{bmatrix}$$

$$\Rightarrow \text{Error} \Rightarrow \mathcal{J}(\omega) \Rightarrow \min_{\omega} \sum_{i=1}^N (y_i - \omega^T \bar{\phi}(x_i))^2 + \frac{\lambda \omega^T \omega}{2}$$

$$A = \begin{bmatrix} \bar{\phi}_m(x_1) & \bar{\phi}_{m+1}(x_1) & \dots & \bar{\phi}_0(x_1) \\ \bar{\phi}_m(x_2) & \bar{\phi}_{m+1}(x_2) & \dots & \bar{\phi}_0(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \bar{\phi}_m(x_N) & \bar{\phi}_{m+1}(x_N) & \dots & \bar{\phi}_0(x_N) \end{bmatrix}$$

$$\Rightarrow \omega = \underbrace{(A^T A)^{-1} A^T y} \Rightarrow \underbrace{(A^T A + \lambda I)^{-1} A^T y}$$

$$\min_w J(w) = \frac{1}{2} \sum_{i=1}^N (y_i - w^T \phi(x_i))^2 + \frac{\lambda}{2} w^T w$$

$w \in \mathbb{R}^m$

$$\nabla_w J(w) = \lambda w + \sum_{i=1}^N -(y_i - w^T \phi(x_i)) \phi(x_i)$$

$w^{(0)} \in \mathbb{R}^m$

$$w^{(1)} = w^{(0)} - \eta_0 \left(\lambda w^{(0)} + \sum_{i=1}^N -(y_i - w^{(0)T} \phi(x_i)) \phi(x_i) \right)$$

$$w^{(2)} = w^{(1)} - \eta_0 \left(\lambda w^{(1)} + \sum_{i=1}^N -(y_i - w^{(1)T} \phi(x_i)) \phi(x_i) \right)$$

Gradient Descent Algo

Initialize $w^0 \in \mathbb{R}^m$

Repeat

$$w^{(k+1)} = w^{(k)} - \eta_k \left(- \sum_{i=1}^N (y_i - w^{(k)T} \phi(x_i)) \phi(x_i) + \lambda w^{(k)} \right)$$

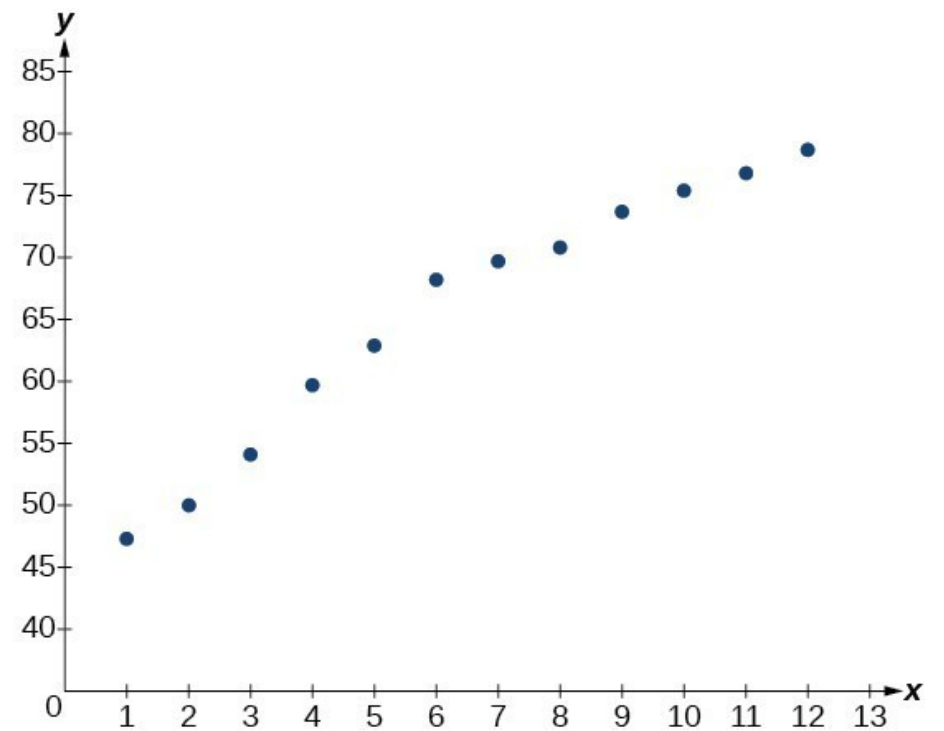
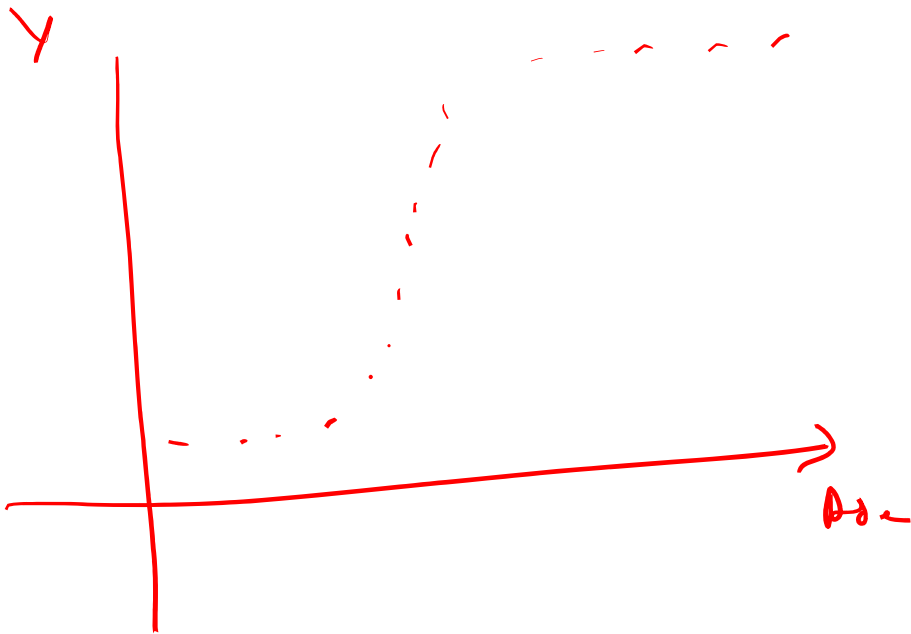
Until $\left\| - \sum_{i=1}^N (y_i - w^{(k)T} \phi(x_i)) \phi(x_i) + \lambda w^{(k)} \right\| \leq \epsilon_{tol}$

~~$$\eta_k = (0.1)^{0.99}$$~~

$$\eta_k = \frac{\eta_{k-1}}{c}$$

$$\eta_k = (\eta_{k-1})^{0.99}$$

Relationship in data



Initialize $w^0 \in \mathbb{R}^m$

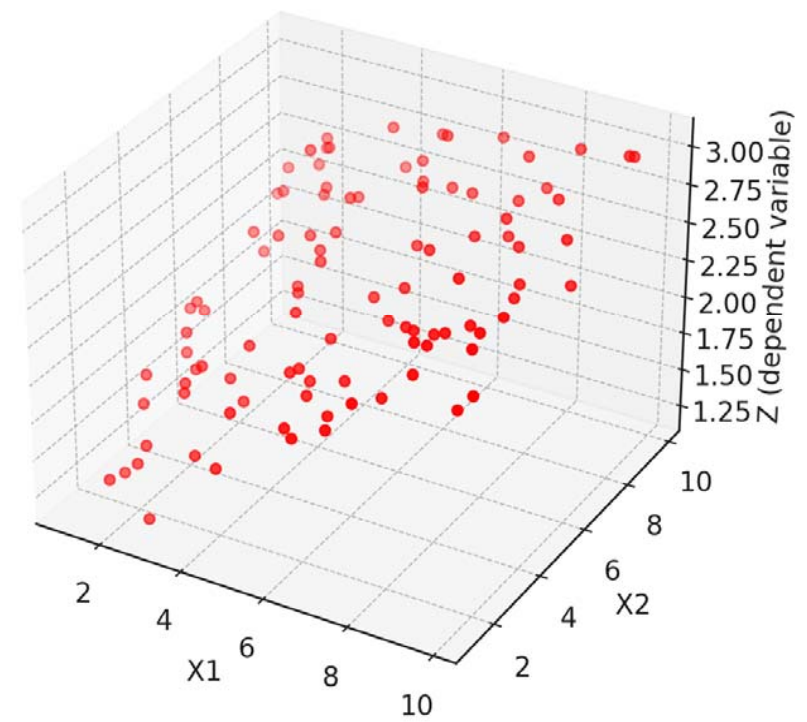
Repeat

Pick a subset B from Training Set T with cardinality K

$$w^{(k+1)} = w^{(k)} - \eta_k \left(\sum_{i \in B} -\varphi(x_i) (y_i - w^{(k)\top} \varphi(x_i)) + \lambda w^{(k)} \right)$$

end

3D Data with Logarithmic Relationship and Noise

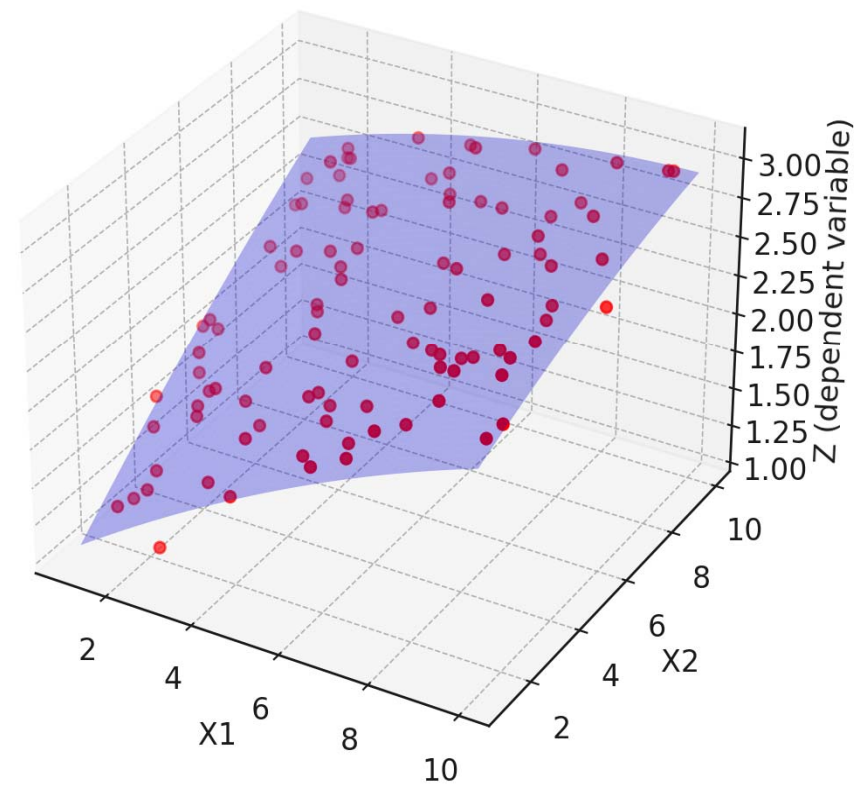


$$\varphi_1(x) = x_1 \checkmark$$

$$\varphi_2(x) = x_2 \checkmark$$

$$\varphi_3(x) = x_1^3 x_2 \checkmark$$

Fitting a Curve to 3D Data with Logarithmic Relationships



$$\Phi(x) = \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \\ \vdots \\ \phi_m(x) \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \quad \left[\exp^{-\frac{1}{2s}} \right]$$

Radial Basis Function (RBF)

- We already have learned about polynomial basis functions
- Another class are radial basis functions (RBF). Typical representatives are Gaussian basis functions

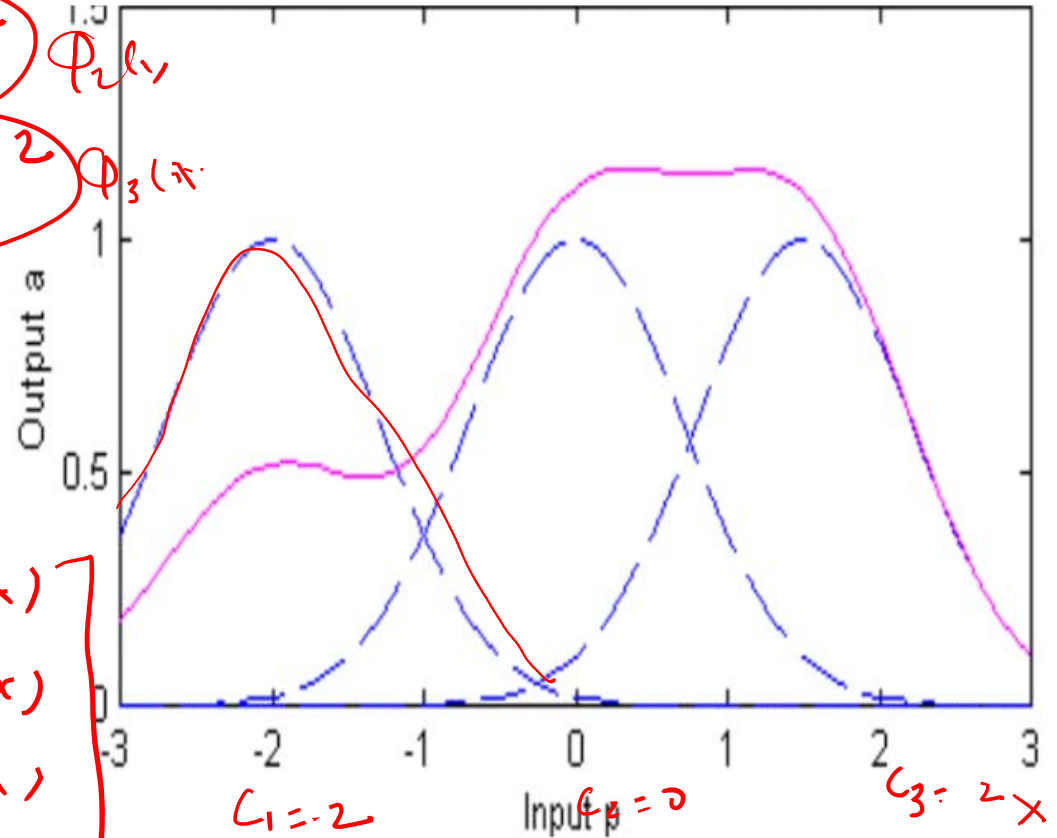
$$\phi_j(x) = \exp \left(-\frac{1}{2s_j^2} \|\mathbf{x} - \mathbf{c}_j\|^2 \right)$$

$$f(x) = \beta_0 + \beta_1 \exp\left(-\frac{1}{2s_1} \|x - c_1\|^2\right) - \phi_1(x)$$

Three RBFs (blue) form $f(x)$ (pink)

$$+ \beta_2 \exp\left(-\frac{1}{2s_2} \|x - c_2\|^2\right) \phi_2(x)$$

$$+ \beta_3 \exp\left(-\frac{1}{2s_3} \|x - c_3\|^2\right) \phi_3(x)$$



$$f(x) = w^T \phi(x)$$

$$w = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}$$

$$\phi(x) = \begin{bmatrix} \phi_1(x) \\ \phi_2(x) \\ \phi_3(x) \\ \phi_4(x) \end{bmatrix}$$

$$c_1 = -2$$

$$s_1 = 2$$

$$c_2 = 0$$

$$s_2 = 2$$

$$c_3 = 2$$

$$s_3 = 2$$

$$\min_w \frac{1}{2} \sum_{i=1}^N (y_i - w^T \phi(x_i))^2 + \frac{\lambda}{2} w^T w$$

$$A = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \phi_3(x_1) & \phi_4(x_1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \phi_3(x_N) & \phi_4(x_N) \end{bmatrix}$$

Testing set: $\{ (x_1, y_1) \dots (x_k, y_k) \}$

$\textcircled{f} \Rightarrow$

$$\text{RMSE} = \sqrt{\frac{1}{k} \sum_{i=1}^k (y_i - f(x_i))^2}$$

$$\frac{\text{SSE}}{\text{SST}} = \frac{\sum_{i=1}^k (y_i - f(x_i))^2}{\sum_{i=1}^k (y_i - \bar{y})^2}$$

$$\text{NMSE} = \frac{\sum_{i=1}^k (y_i - \bar{y})^2}{\sum_{i=1}^k (y_i - f(x_i))^2}$$

$$\text{MAE} = \frac{1}{k} \sum_{i=1}^k |y_i - f(x_i)|$$