# ED5340 - Data Science: Theory and Practise

L18 - Linear Regression: Multivariate

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Course web page: https://ed.iitm.ac.in/~raman/datascience.html

Moodle page: Available at https://courses.iitm.ac.in/

#### Univariate

- Ground truth data Input feature / output  $(\mathbf{x}, \mathbf{y})$  are the knowns
- Use a model / hypothesis as h(w)
- Develop an error / cost / loss function  $J(w) = J(\mathbf{y}, \bar{\mathbf{y}}) = J(\mathbf{y}, h(w))$
- The weights are identified by
  - $\min J(w)$
- Essentially, ML problem is now reduced to an optimization problem.
- Weights are identified using Optimization.

#### **Univariate case**

- Ground truth data Input feature / output (x, y) are the knowns
- Use a model / hypothesis as h(w) and cost function J(w)

Input (x)

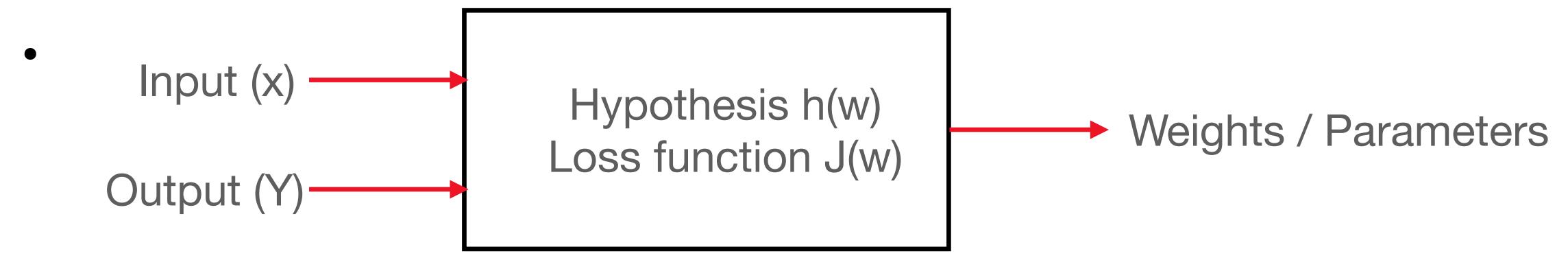
Hypothesis h(w)

Loss function J(w)

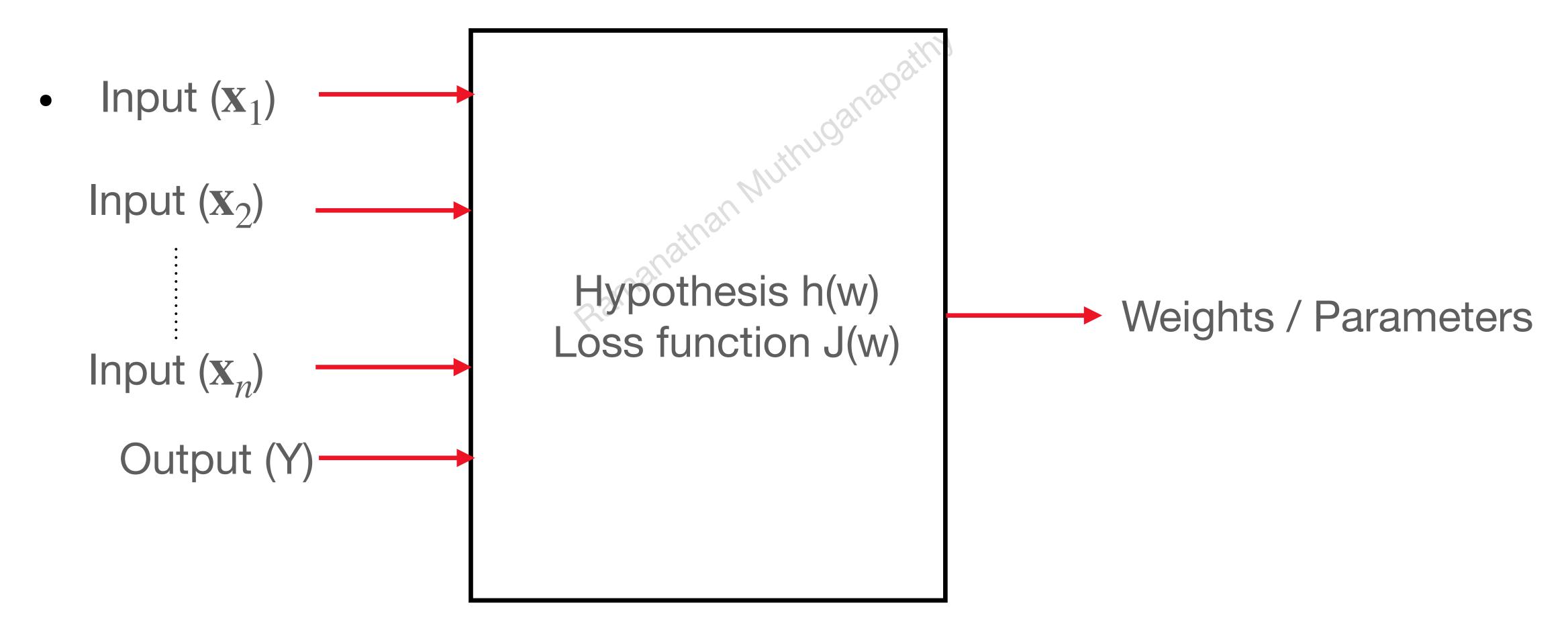
Weights / Parameters

#### Multivariate case

- Ground truth data Input feature / output  $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \dots \mathbf{x}_n, \mathbf{y})$  are the knowns n features
- $\mathbf{x}_1$  Size,  $\mathbf{x}_2$  BA,  $\mathbf{x}_3$  Distance to school,  $\mathbf{x}_4$  To hospital,  $\mathbf{x}_5$  maintenance etc..
- Use a model / hypothesis as h(w) and cost function J(w)



Multivariate case (n features)



#### **Supervised Leaning**

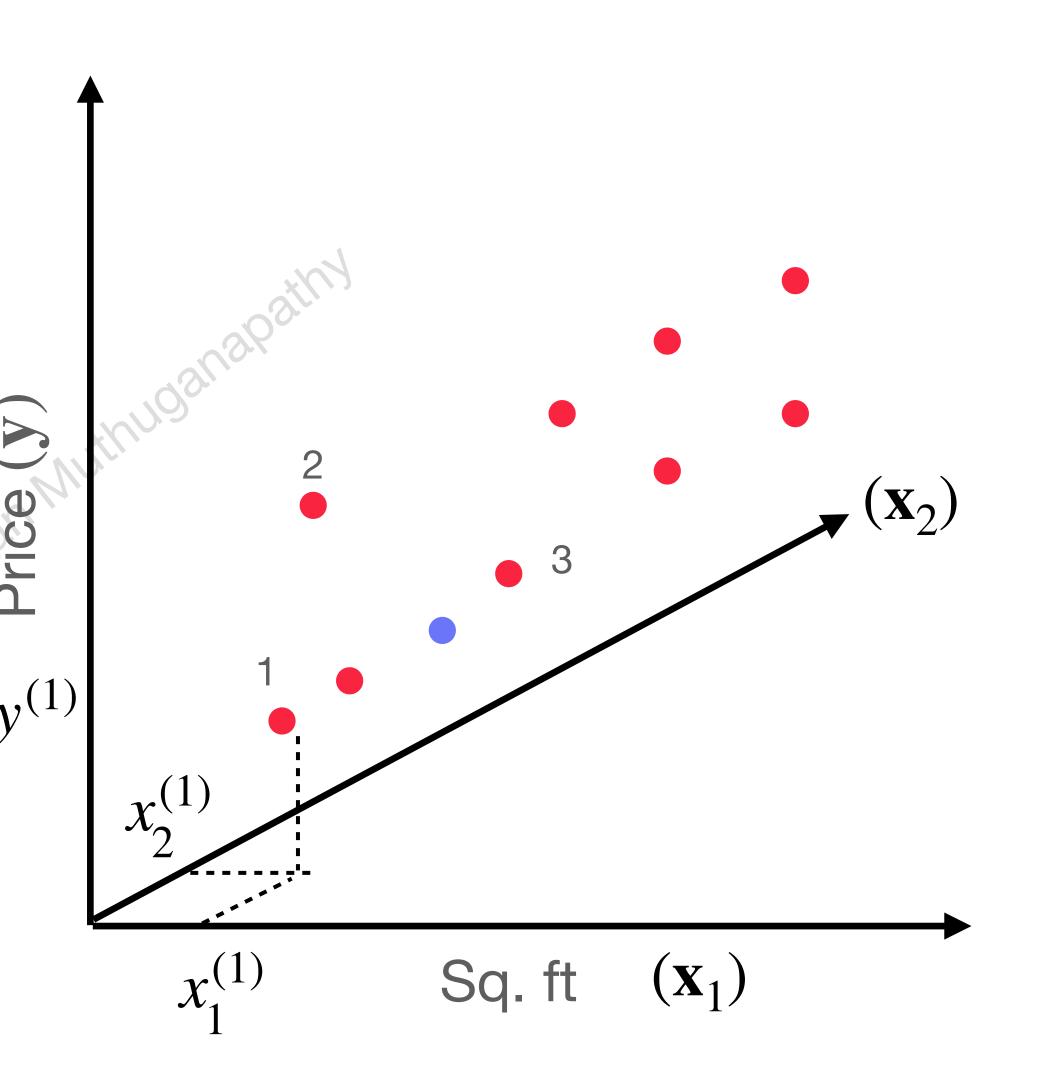
• Each feature will have *m* training samples

• 
$$\mathbf{x}_1 = (x_1^{(1)}, x_1^{(2)}, x_1^{(3)}, \dots, x_1^{(m)})$$

• 
$$\mathbf{x}_{1}$$
 ( $x_{1}$ ,  $x_{1}$ ,  $x_{1}$ ,  $x_{1}$ , ...,  $x_{1}$ )
•  $\mathbf{x}_{2} = (x_{2}^{(1)}, x_{2}^{(2)}, x_{2}^{(3)}, \dots, x_{2}^{(m)})$ 
•  $\mathbf{x}_{2}$  ( $\mathbf{x}_{2}$ )

• 
$$\mathbf{x}_n = (x_n^{(1)}, x_n^{(2)}, x_n^{(3)}, \dots, x_n^{(m)})$$

• 
$$\mathbf{y} = (y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(m)})$$



#### n dimensional coordinates

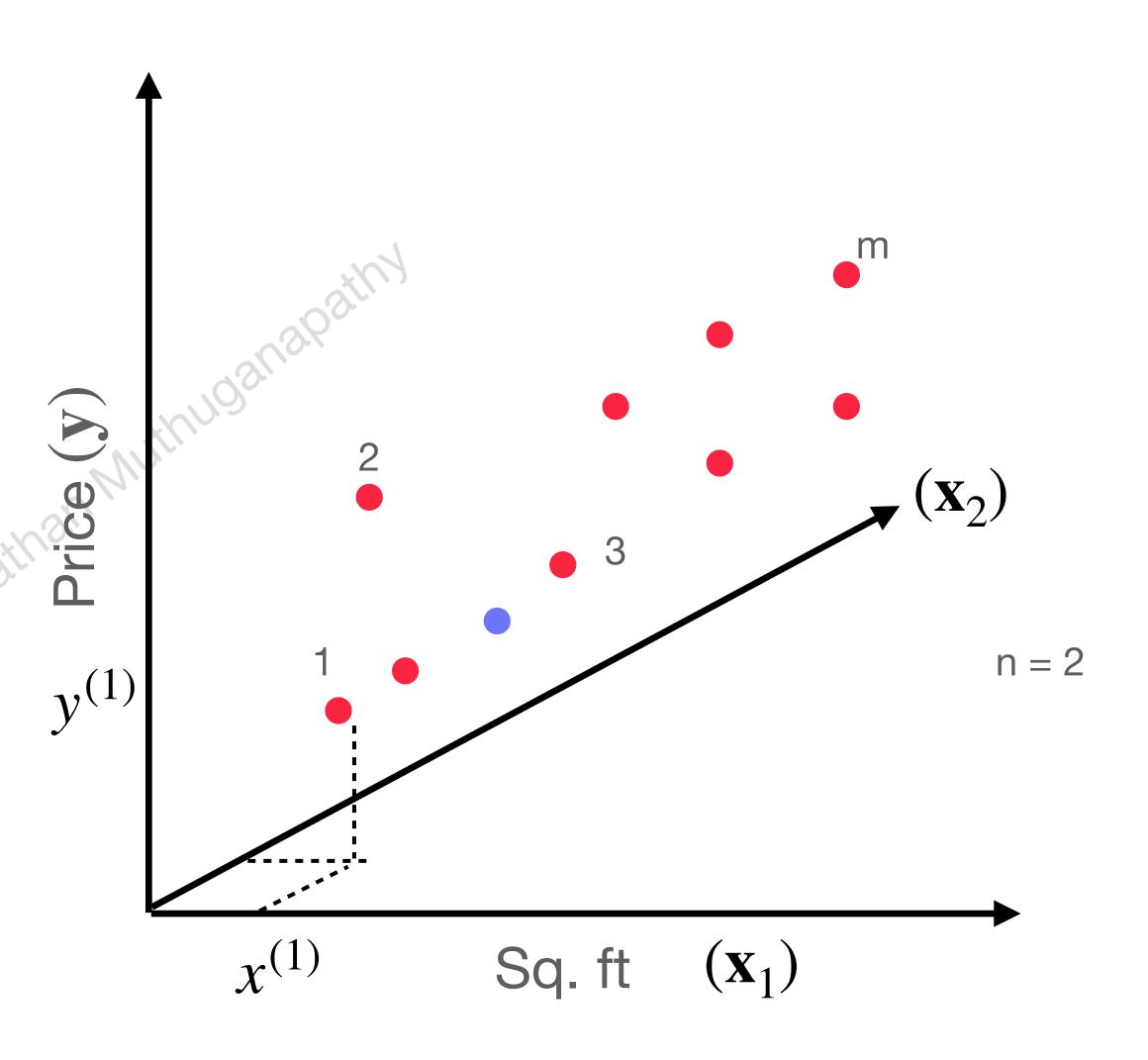
• Each training sample will come from *n* features (*n* dimensional coordinates)

• 
$$(x_1^{(1)}, x_2^{(1)}, x_3^{(1)}, \dots, x_n^{(1)})$$

• 
$$(x_1^{(2)}, x_2^{(2)}, x_3^{(2)}, \dots x_n^{(2)})$$

• 
$$(x_1^{(m)}, x_2^{(m)}, x_3^{(m)}, \dots, x_n^{(m)})$$

• 
$$\mathbf{y} = (y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(m)})$$



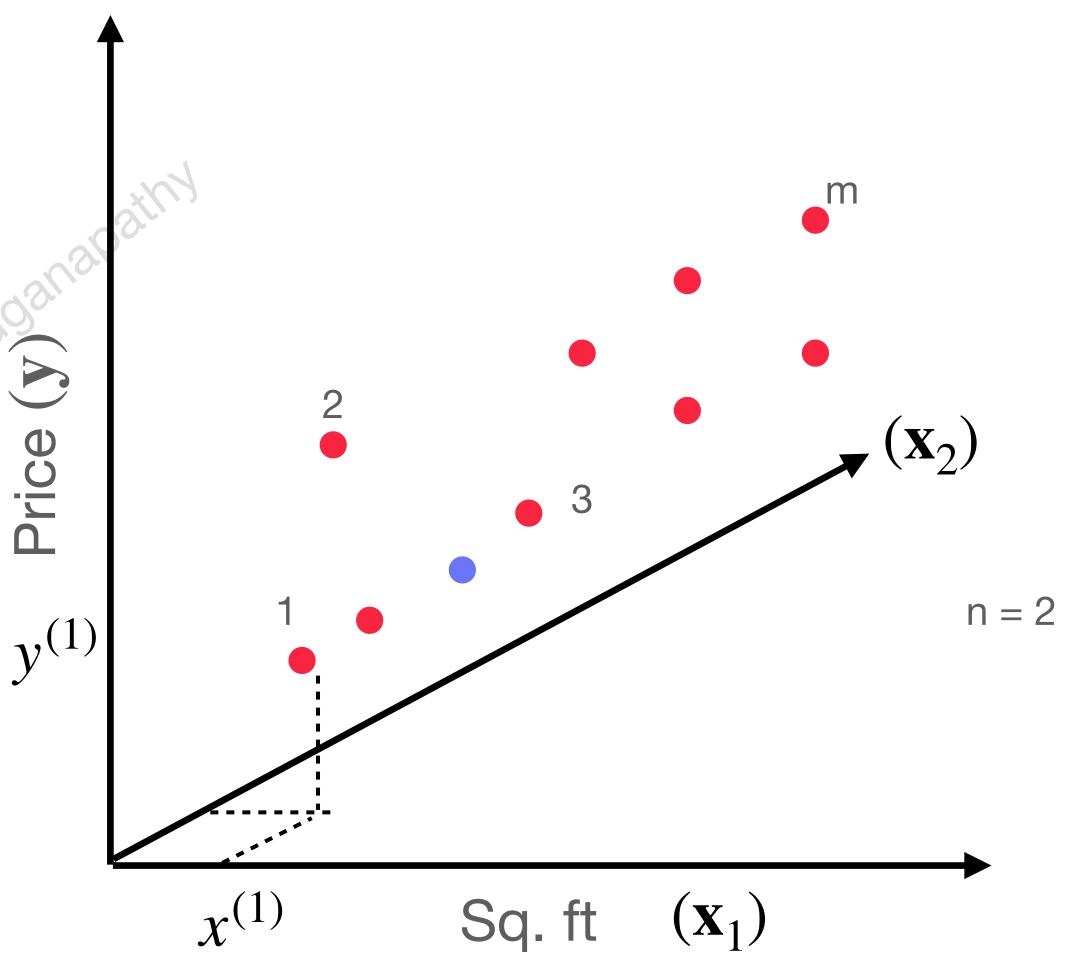
## Sample data

#### m samples each with n features

sample number	Size X <sub>1</sub>	<b>BA X</b> <sub>2</sub>	Maintanence X <sub>3</sub>	y <sup>(i)</sup> Price
$(x_1^{(1)}, x_2^{(1)}, x_3^{(1)})$	1000	800	2.5	70
$(x_1^{(2)}, x_2^{(2)}, x_3^{(2)})$	1500	1250	3.0	85
$(x_1^{(m)}, x_2^{(m)}, x_3^{(m)})$	800	400	3.5	55

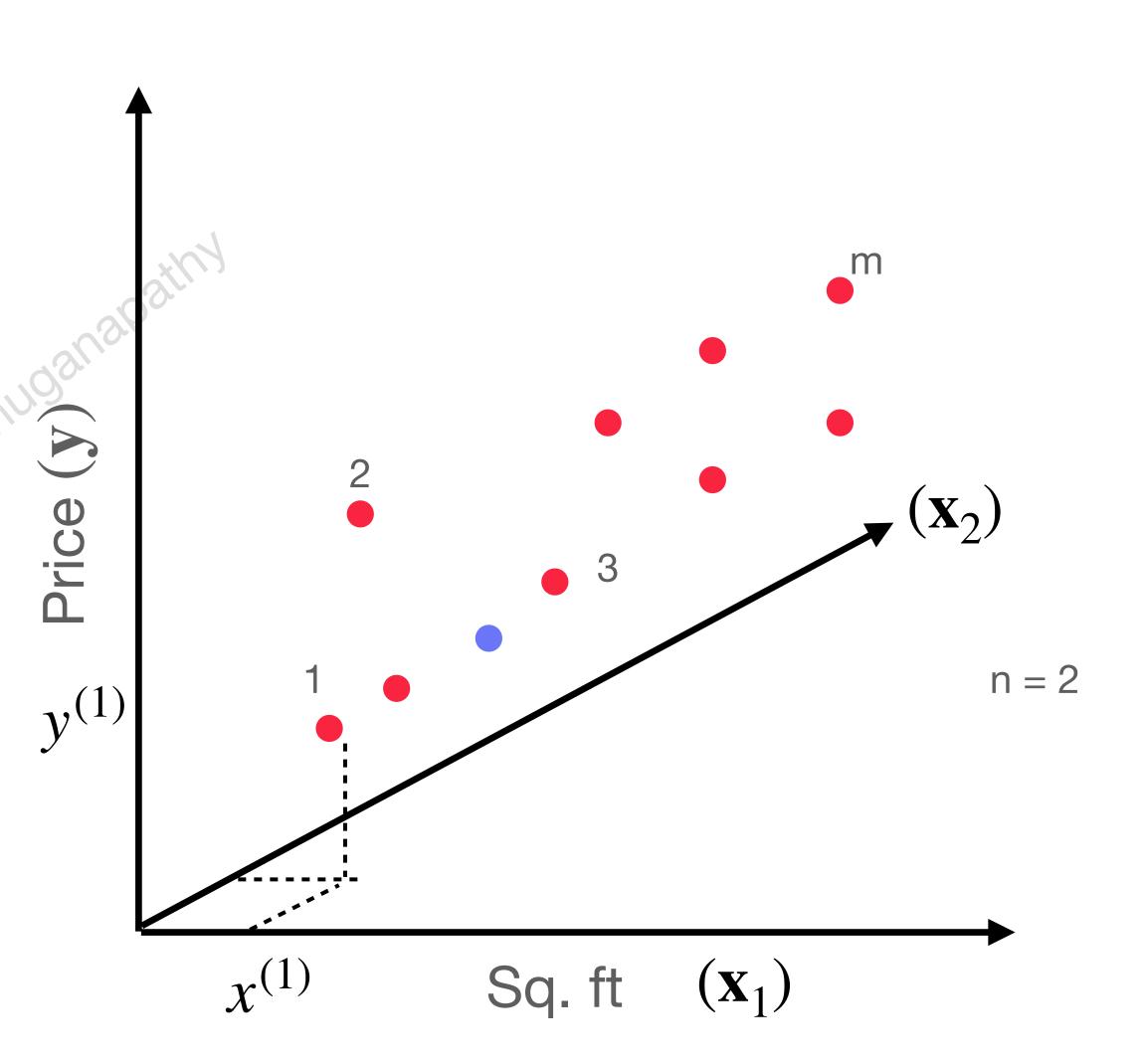
#### Goal: Approximation that fits the data

- Look at the data, hyperplane fit is carried out!
- $h_w(x) = w_0 + w_1 x_1 + w_1 x_2 + w_3 x_3$
- Goal: Determine weights  $(w_0, w_1, w_2, \dots, w_n)$



#### **Generalized form**

- Look at the data, hyperplane fit is carried out!
- $h_w(x) = w_0 x_0 + w_1 x_1 + w_1 x_2 + w_3 x_3$
- $x_0 = 1$
- $h_w(x) = \mathbf{w}^T \mathbf{x} \text{ (or } = \mathbf{x}^T \mathbf{w})$

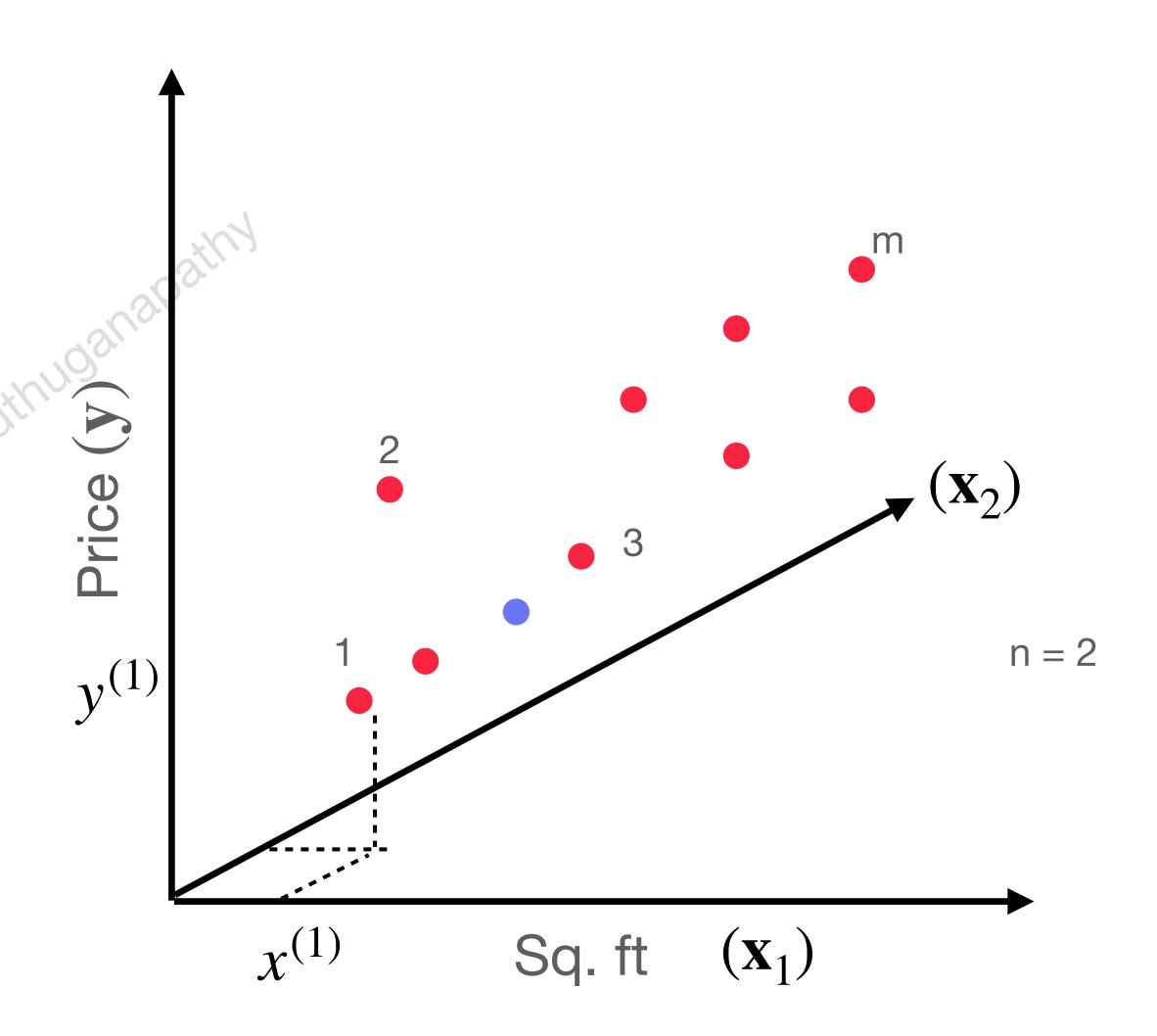


#### **Generalized form**

• 
$$h_w(x) = \mathbf{w}^T \mathbf{x}$$
 (or  $= \mathbf{x}^T \mathbf{w}$ )

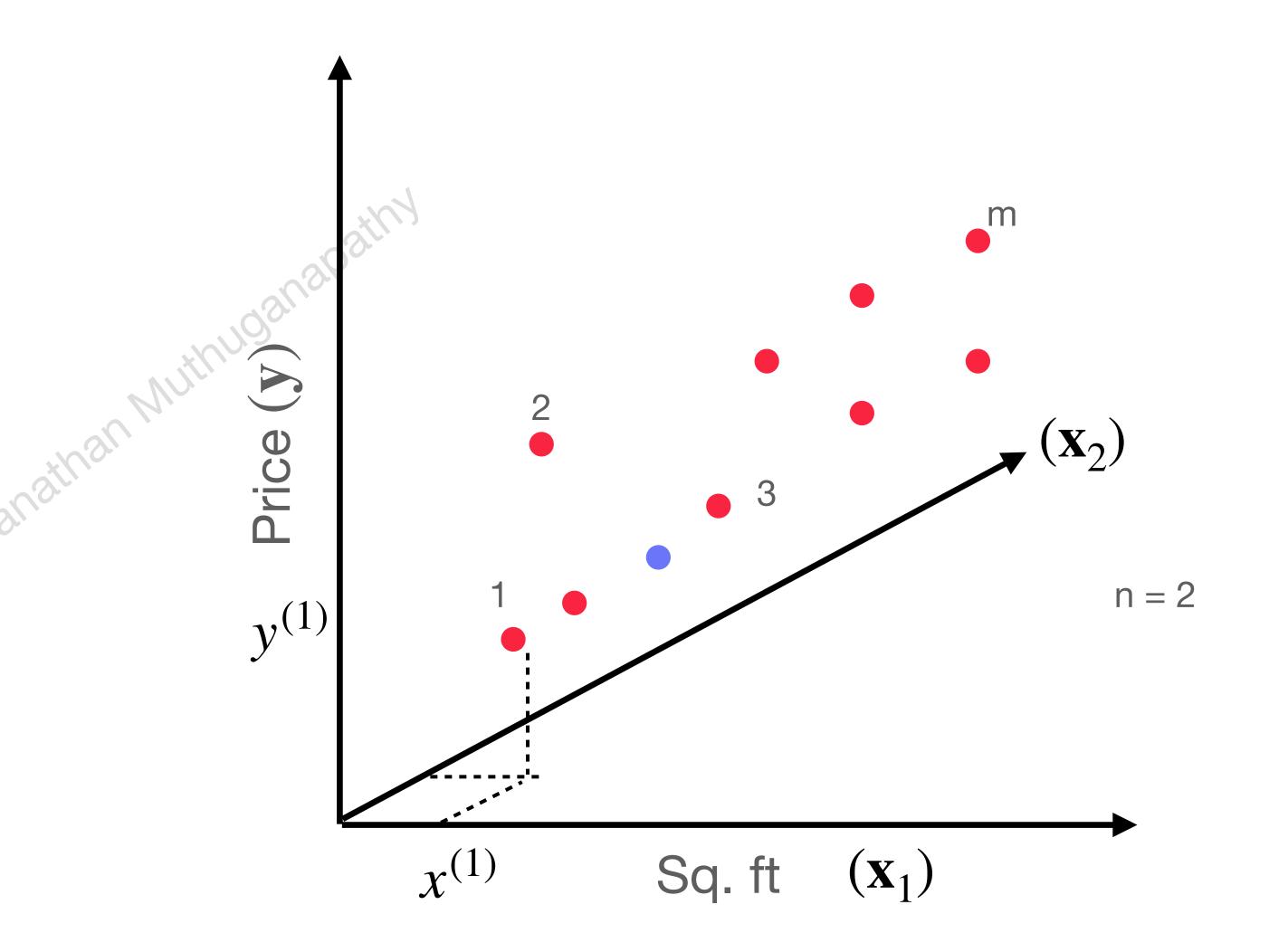
• 
$$\mathbf{w}^T = \begin{bmatrix} w_0 & w_1 & w_2 & w_3 \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix}$$



#### **Generalized form**

$$\mathbf{x} = \begin{bmatrix} 1 & 1 & 1 \\ x_1^{(1)} & x_1^{(2)} & x_1^{(3)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} \\ x_3^{(1)} & x_3^{(2)} & x_3^{(3)} \end{bmatrix}$$



#### **Predicted values**

• 
$$\mathbf{y} = (y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(m)})$$

• 
$$\bar{\mathbf{y}} = (\bar{y}^{(1)}, \bar{y}^{(2)}, \bar{y}^{(3)}, \dots \bar{y}^{(m)})$$

• 
$$\bar{y}_j^{(i)} = h_w(x_j^{(i)}) = w_0 x_j^{(i)} + w_1 x_j^{(i)} + w_2 x_j^{(i)} + w_3 x_j^{(i)}$$

- Goal: Determine weights  $(w_0, w_1, w_2, w_3)$
- i 1 to m (training samples), j = 1 to n (features)

#### Minimize the cost function

$$J(w) = \sum_{i=1}^{m} \frac{1}{2m} (w_0 x_j^{(i)} + w_1 x_j^{(i)} + w_2 x_j^{(i)} + w_3 x_j^{(i)} - y^{(i)})^2$$
 • min  $J(w)$ 

•  $\min J(w)$ 

#### **Gradient descent**

• Find 
$$\nabla J(w_0, w_1, w_2, w_3) = \left(\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}, \dots\right)$$

$$\frac{\partial J}{\partial w_0} = \frac{1}{m} \sum_{i=1}^{m} (w_0 x_0^{(i)} + w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} - y^{(i)}) x_0^{(i)}$$

$$\frac{\partial J}{\partial w_1} = \frac{1}{m} \sum_{i=1}^{m} (w_0 x_0^{(i)} + w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} - y^{(i)}) x_1^{(i)}$$

$$\frac{\partial J}{\partial w_2} = \frac{1}{m} \sum_{i=1}^{m} (w_0 x_0^{(i)} + w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} - y^{(i)}) x_2^{(i)}$$

$$\frac{\partial J}{\partial w_3} = \frac{1}{m} \sum_{i=1}^{m} (w_0 x_0^{(i)} + w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} - y^{(i)}) x_3^{(i)}$$

#### Gradient descent update

$$\frac{\partial J}{\partial w_j} = \frac{1}{m} \sum_{i=1}^m (w_0 x_0^{(i)} + w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)} - y^{(i)}) x_j^{(i)}$$

$$w_j^{k+1} = w_j^k - \alpha_k \frac{\partial J}{\partial w_j}$$

$$w_j^{k+1} = w_j^k - \alpha_k \frac{\partial J}{\partial w_j}$$

#### Gradient descent update

$$\frac{\partial J}{\partial w_j} = \frac{1}{m} \sum_{i=1}^{m} (h_w(x) - y^{(i)}) x_j^{(i)}$$

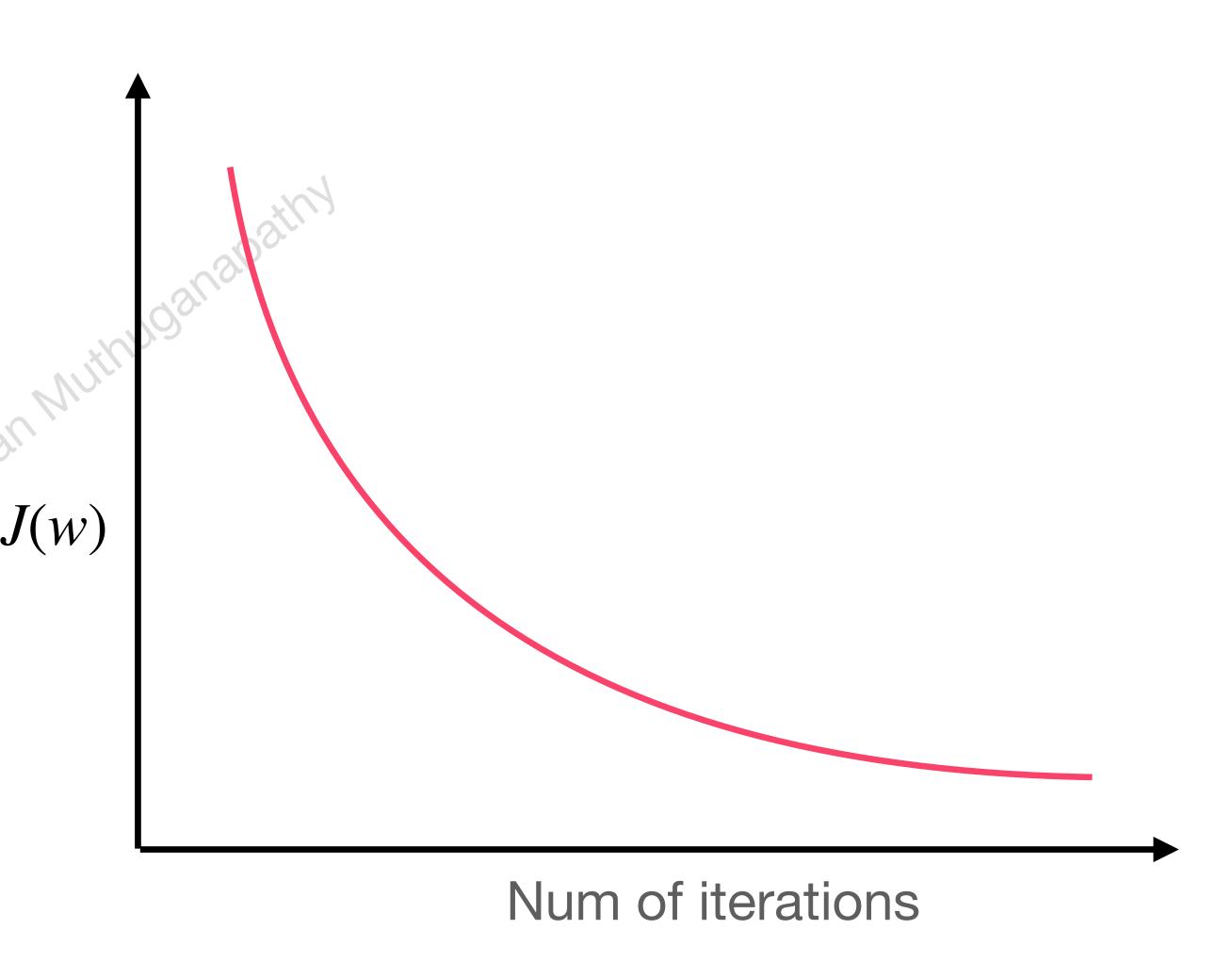
$$w_j^{k+1} = w_j^k - \alpha_k \frac{\partial J}{\partial w_j}$$

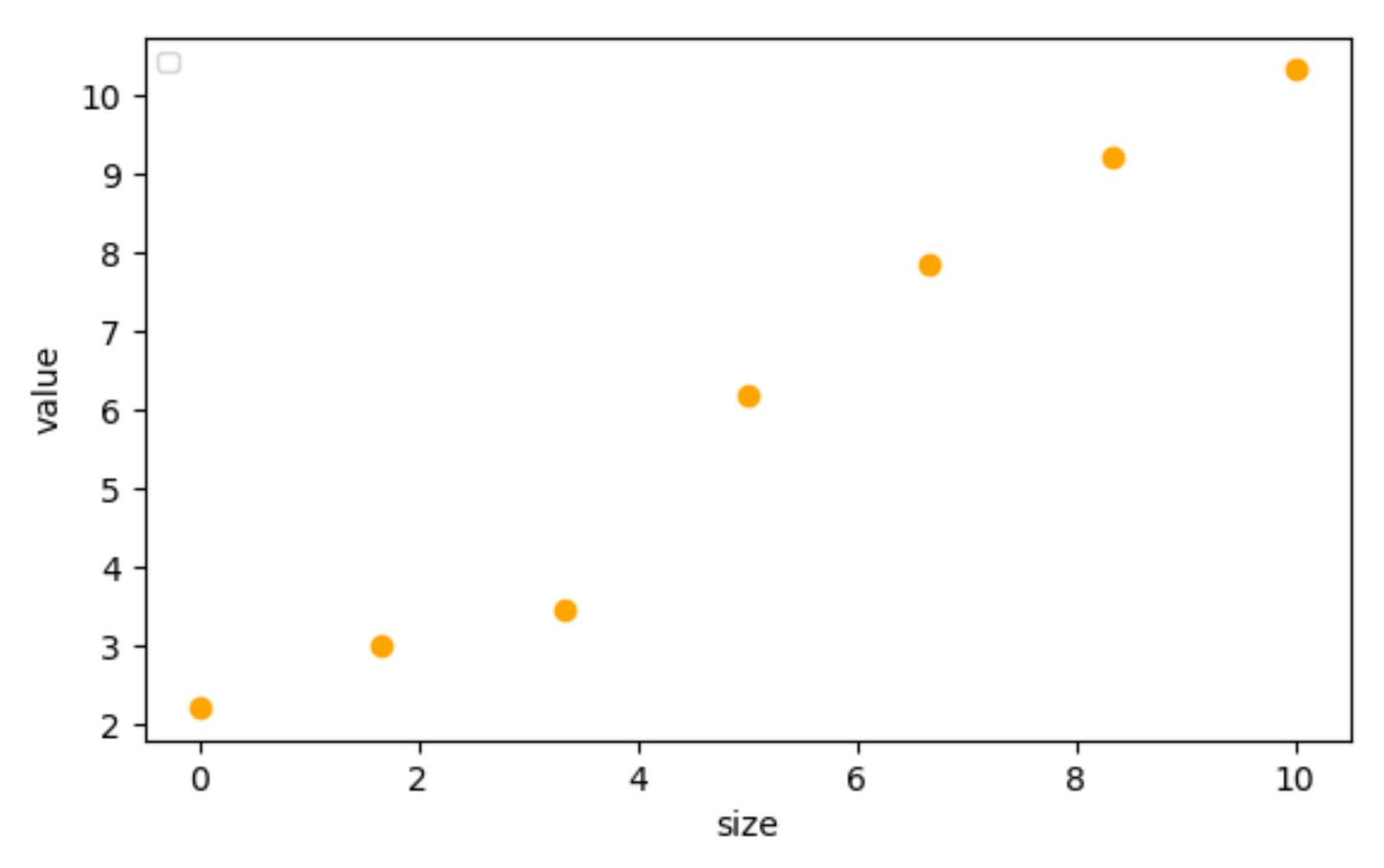
## Feature scaling Normalising the features

- Features are on a similar scale
- Normalise the features (0 to 1)
- Normalise the features (-1 to 1) around that range
- Normalising over mean

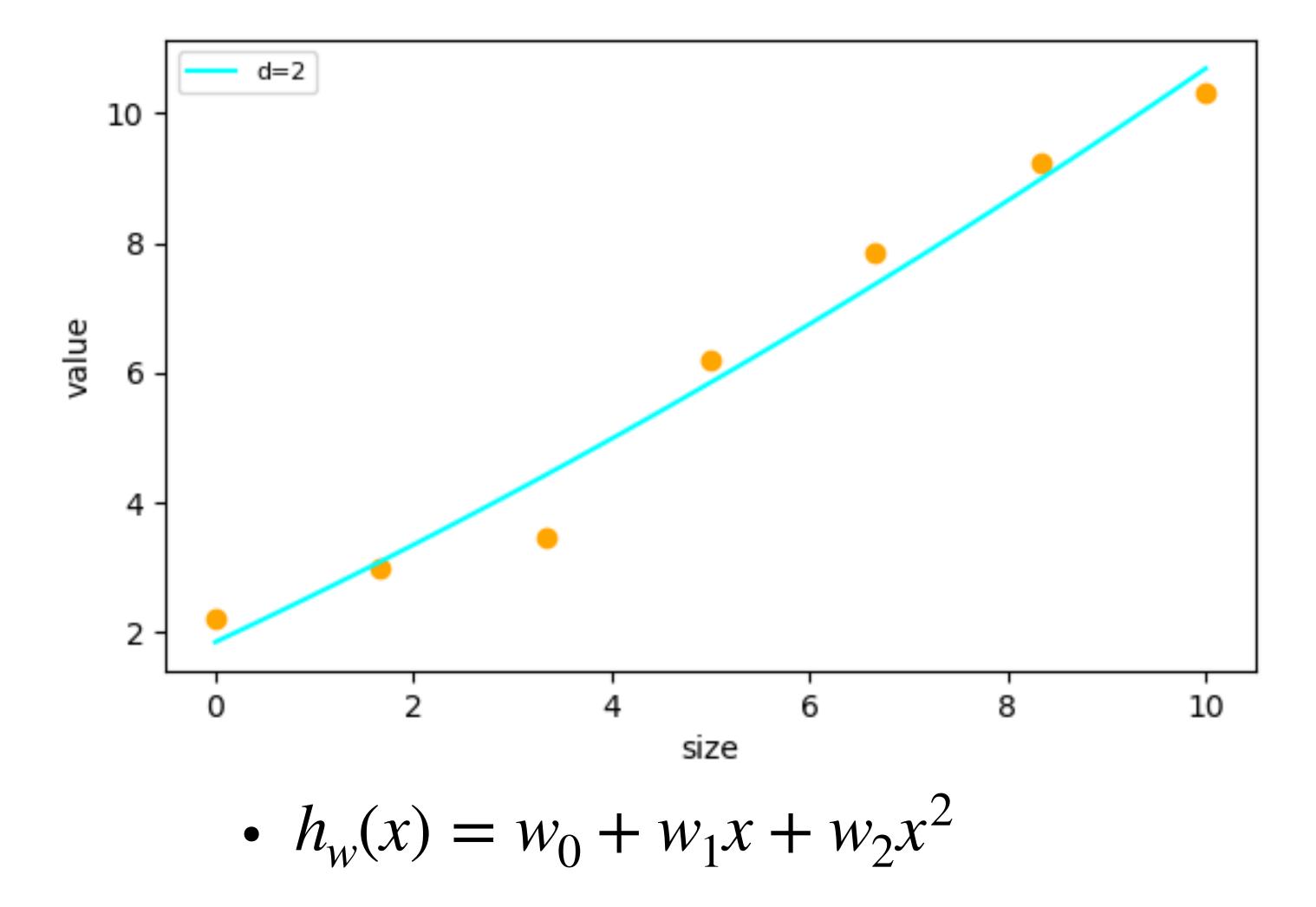
## S. Gradient Descent Debugging

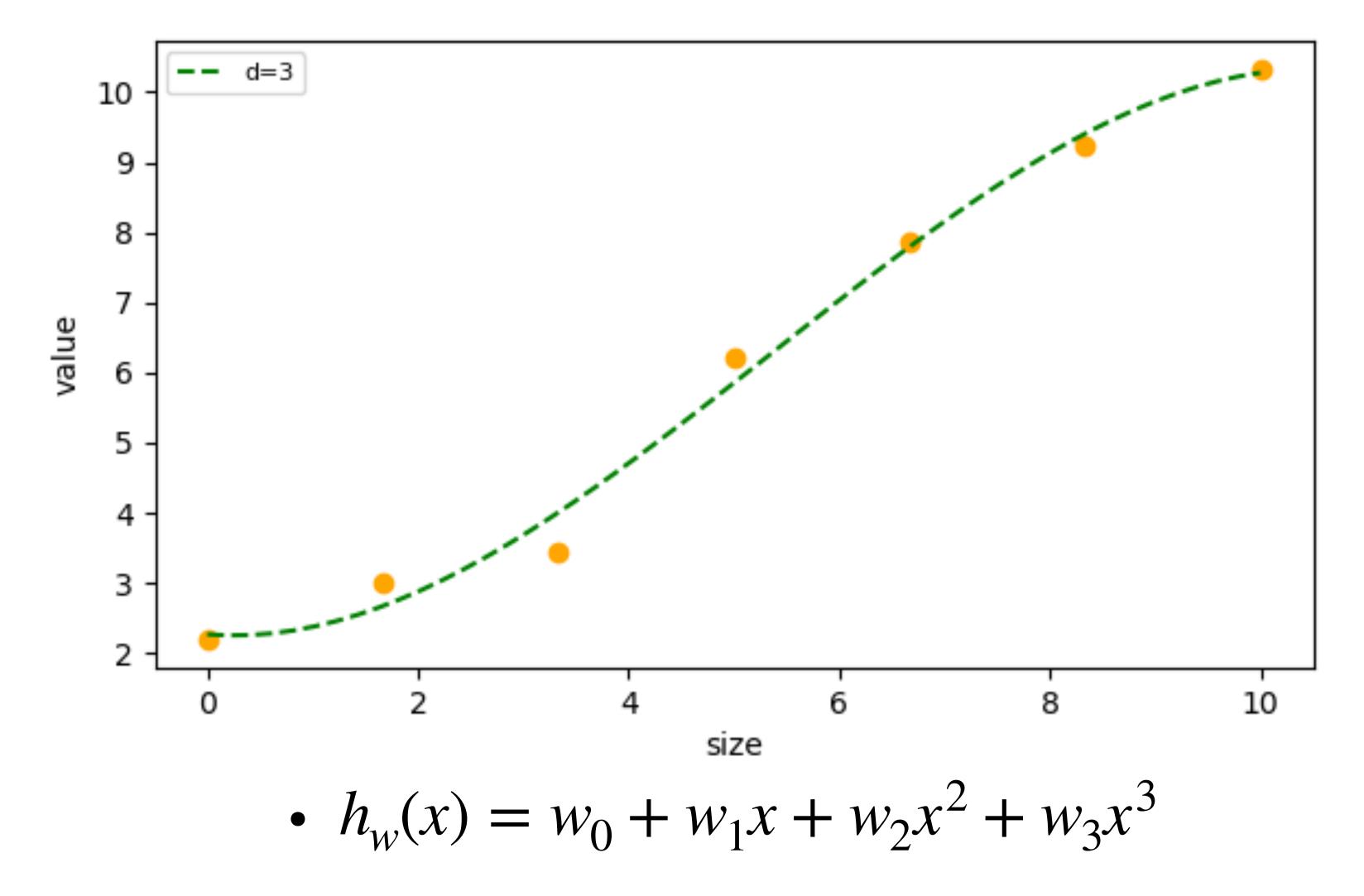
- Plot k (iteration) vs J (Cost)
- $\alpha_k$  too small, slow convergence
- $\alpha_k$  too large, could also be another issue
- Use line search to find  $\alpha_k$

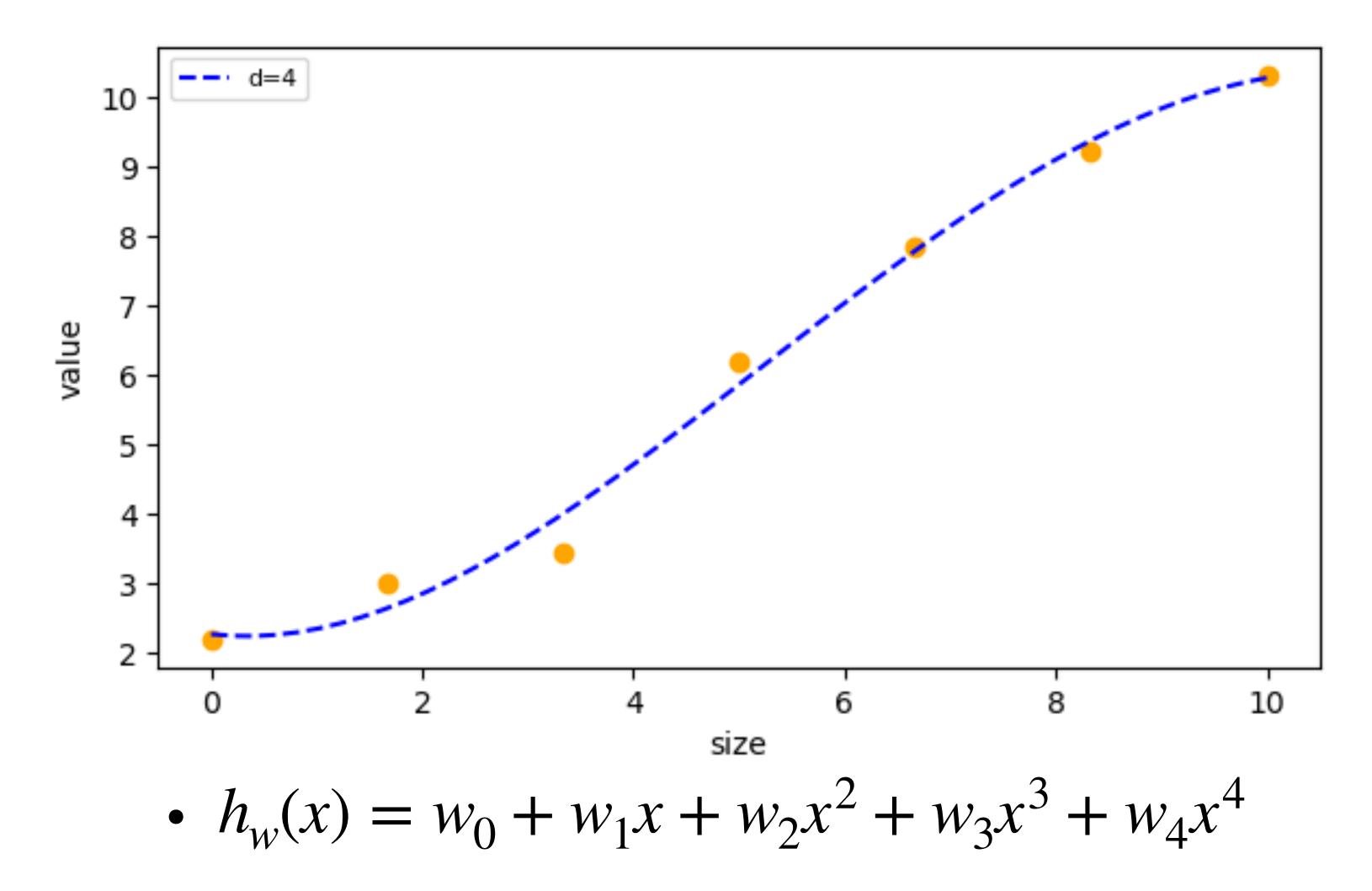


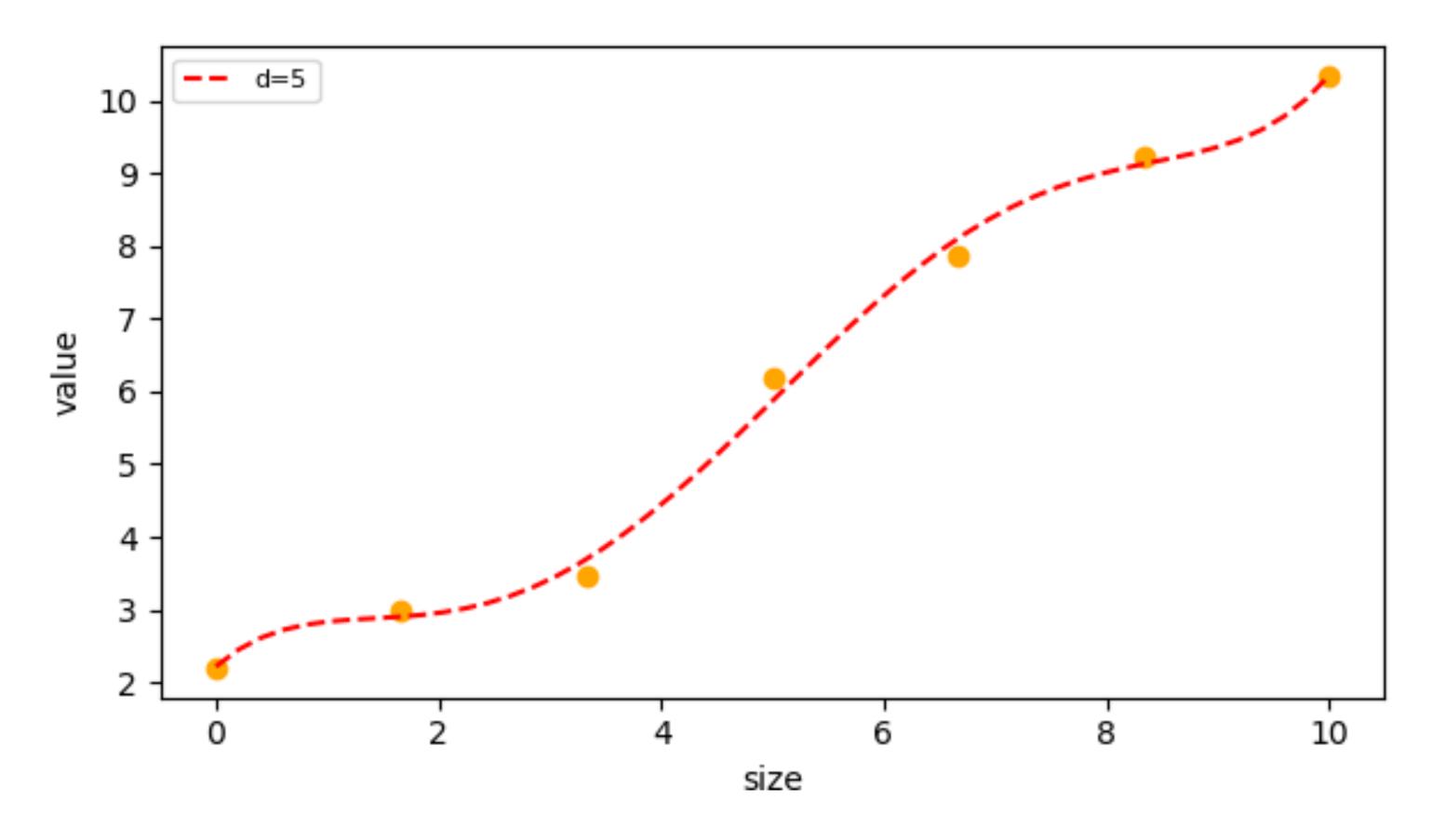


Imagine the data points

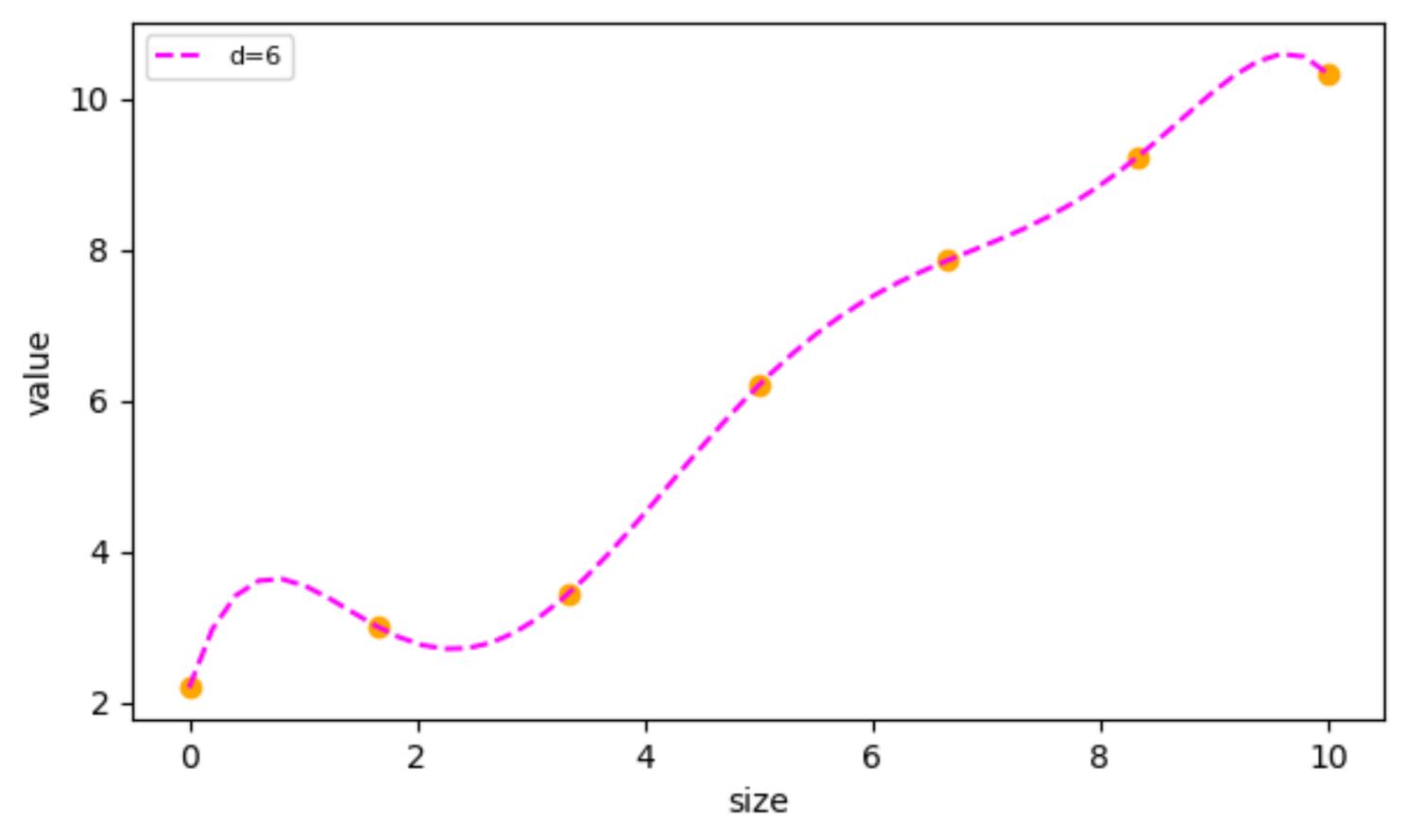








• 
$$h_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$$

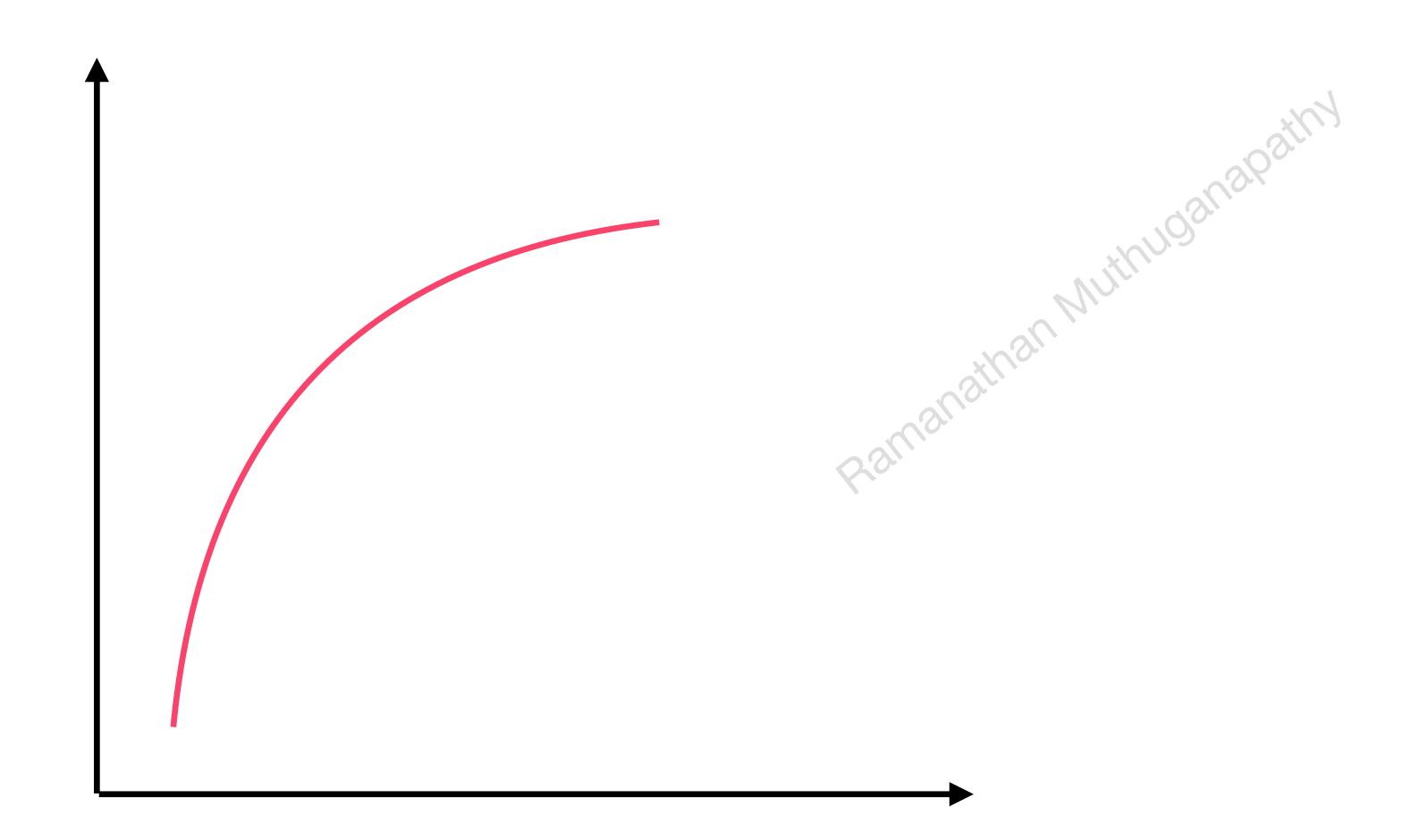


• 
$$h_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5 + w_6 x^6$$

- The fit is seemingly the best!
- Oscillations starts for higher degree polynomials
- Given the data, find the weights using optimisation

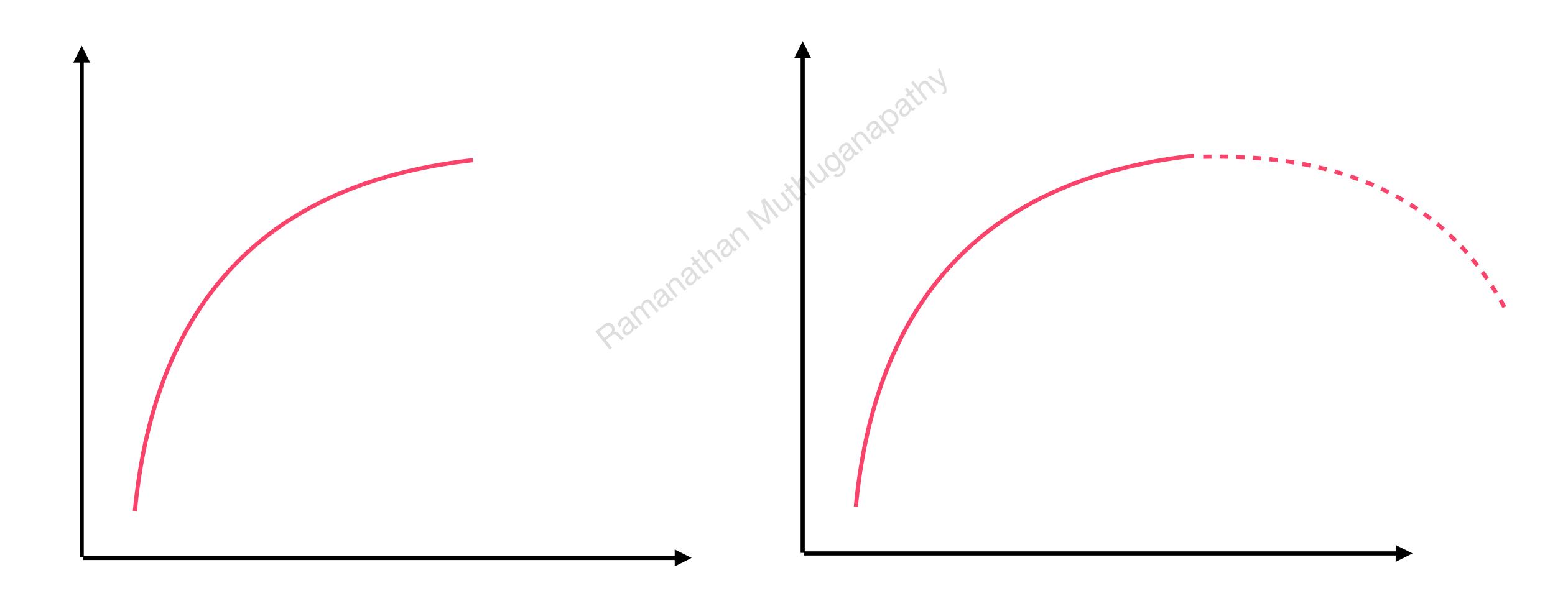
#### Other issues...

#### E.g. Quadratic



#### Other issues...

#### E.g. Quadratic



## Various possible models

• 
$$h_w(x) = w_0 + w_1 x + w_2 x^2$$

• 
$$h_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

- — —
- — –
- —

• 
$$h_w(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5 + w_6 x^6$$

## Various possible models - multivariate

#### Two features

• 
$$h_w(x) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2$$

• 
$$h_w(x) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2$$
  
•  $h_w(x) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + w_4 x_1^2 + w_5 x_2^2$