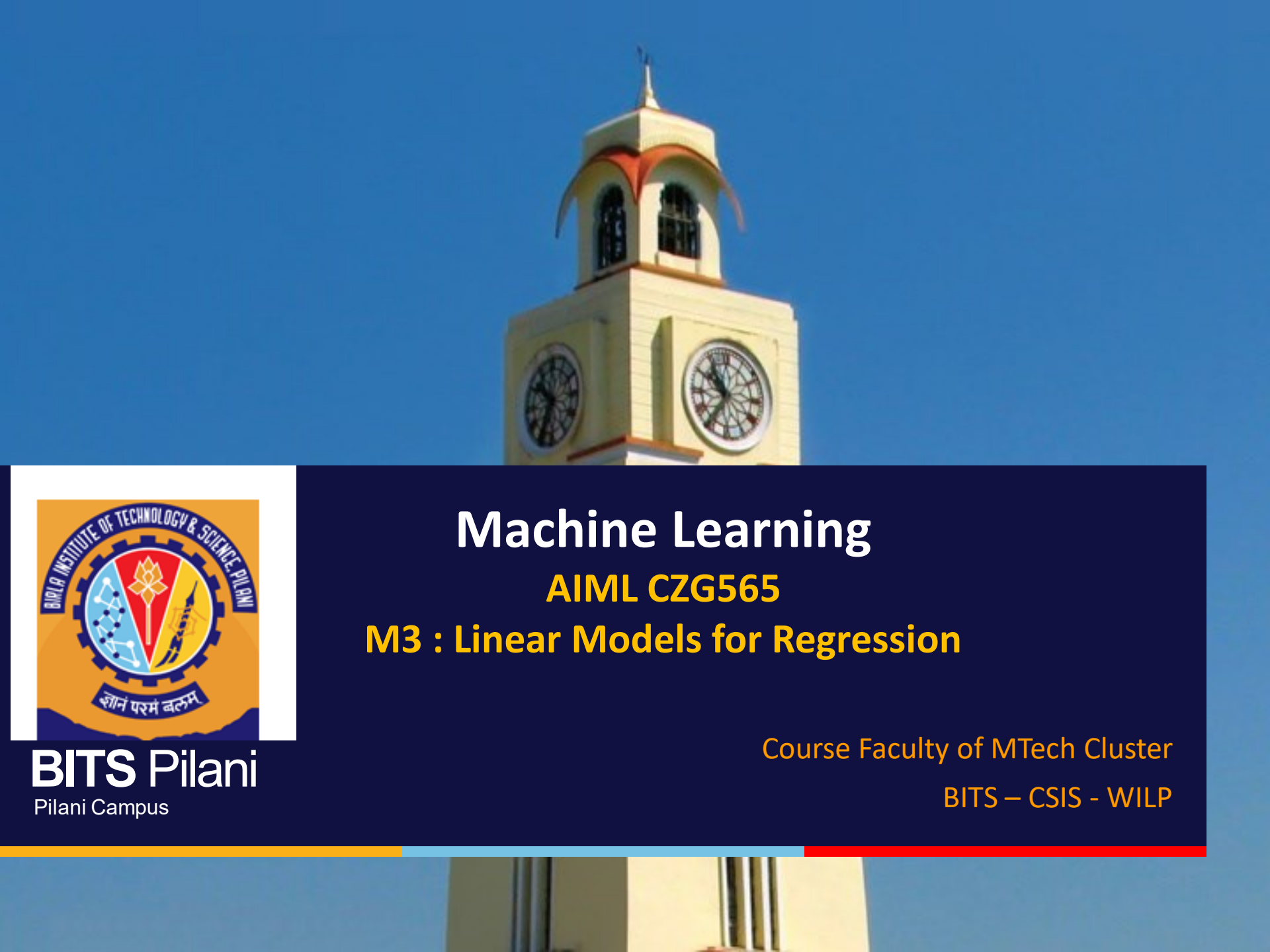


Machine Learning

AIML CZG565

M3 : Linear Models for Regression

Course Faculty of MTech Cluster

BITS – CSIS - WILP

BITS Pilani

Pilani Campus

Machine Learning

Disclaimer and Acknowledgement

- The content for these slides has been obtained from books and various other source on the Internet
- We here by acknowledge all the contributors for their material and inputs.
- We have provided source information wherever necessary
- Students are requested to refer to the textbook w.r.t detailed content of the presentation deck shared over canvas
- We have reduced the slides from canvas and modified the content flow to suit the requirements of the course and for ease of class presentation

Source: "Probabilistic Machine Learning, An Introduction", Kevin P. Murphy, Slides of Prof.Sugata, Prof. Chetana from BITS Pilani, Prof. Raja vadhana from BITS Pilani , CS109 and CS229 stanford lecture notes and many others who made their course materials freely available online.

Course Plan

M1	Introduction
M2	Machine learning Workflow
M3	Linear Models for Regression
M4	Linear Models for Classification
M5	Decision Tree
M6	Instance Based Learning
M7	Support Vector Machine
M8	Bayesian Learning
M9	Ensemble Learning
M10	Unsupervised Learning
M11	Machine Learning Model Evaluation/Comparison

Agenda

- Linear Model for Regression
- Direct solution vs Iterative Method
- Gradient Descent **(Introduction)**
- Linear Basis Function
- Notion of Bias vs Variance

Linear Regression

Inductive Learning Hypothesis : Interpretation

- Target Concept
- Discrete : f(x) ∈ {Yes, No, Maybe} Classification
- Continuous : f(x) ∈ [20-100] Regression
- Probability Estimation : f(x) ∈ [0-1]

Sky	AirTemp	Altitude	Wind	Water	Forecast	Humidity
Sunny	Warm	Normal	Strong	Warm	Same	60
Sunny	Warm	High	Strong	Warm	Same	75
Rainy	Cold	High	Strong	Warm	Change	70
Sunny	Warm	High	Strong	Cool	Change	45

Regression – Introduction

Supervised Learning: Regression

Wish to learn a function f : X → Y, where predicted output Y is real, given the n real training instances $\{<x^1,y^1>\ldots<x^n,y^n>\}$.

Examples include

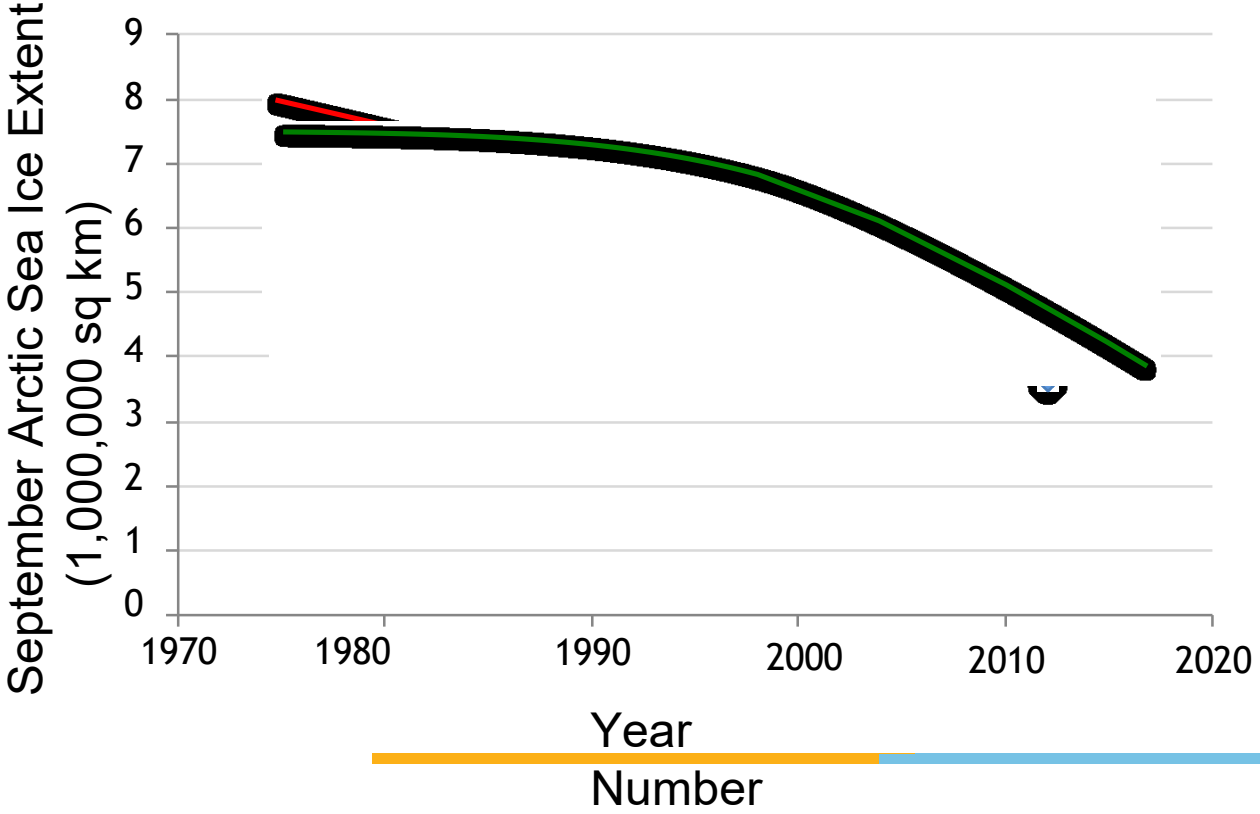
- predict weight from gender, height, age, …
- Predict house price from locality, area, income, …
- predict Google stock price today from Google, Yahoo, MSFT prices yesterday
- predict each pixel intensity in robot's current camera image, from previous image and previous action

Formal Representation: Interpretation

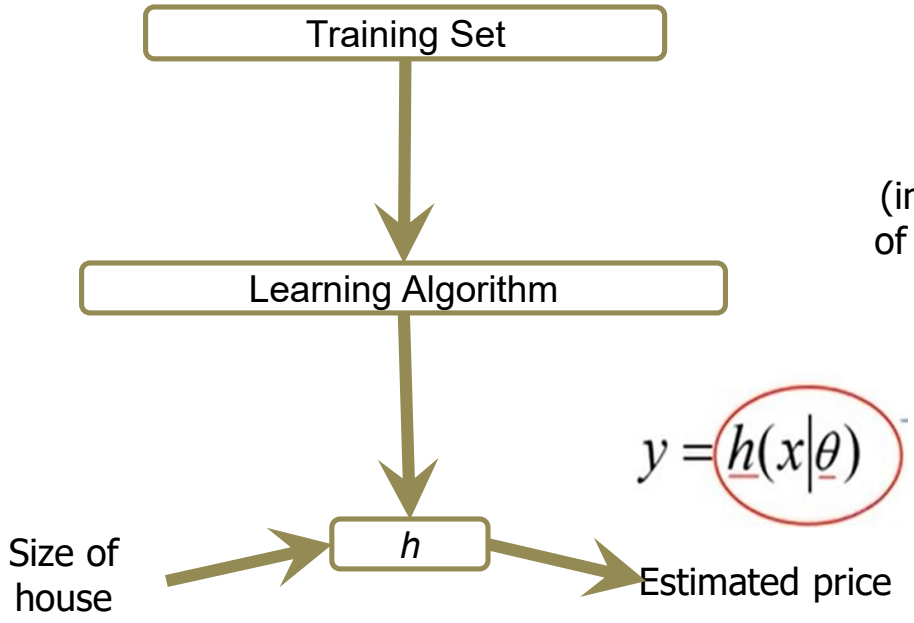
Supervised Learning: Regression

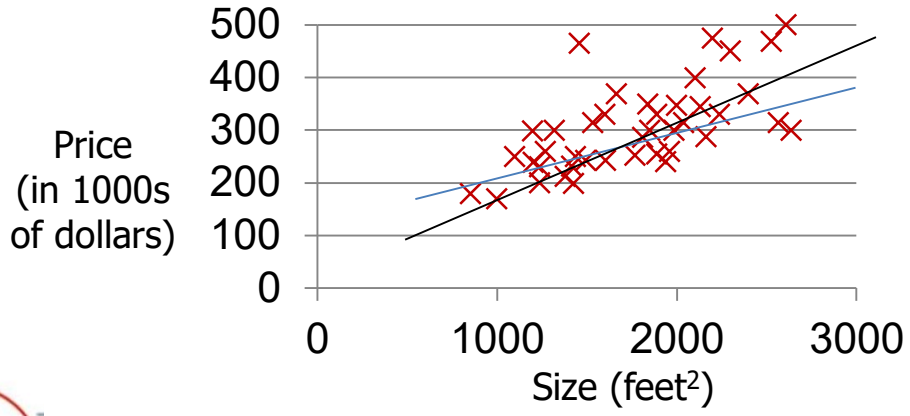
GOAL : Previously unseen records should be assigned a value as accurately as possible.

- Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
- Learn a function $f(x)$ to predict y given x
  - y is real-valued



Machine Learning Process : Interpretation





Size in feet² (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
…	…

Hypothesis: [redacted]

θ_i's : Parameters

h(.) : Model

How to choose θ_i's ?

Types of Regression Models

simple regression model

(Education) x ⟶ y (Income)

multiple regression model

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x,$$

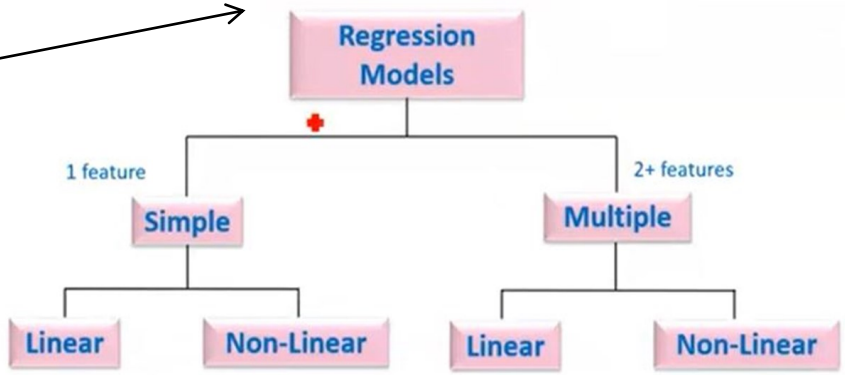
(Education) x_1

(Soft Skills) x_2

(Experience) x_3

(Age) x_4

y (Income)



- Hypothesis:

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j$$

Assume $x_0 = 1$

Learning the Model Parameters

Closed Form Solution Approach

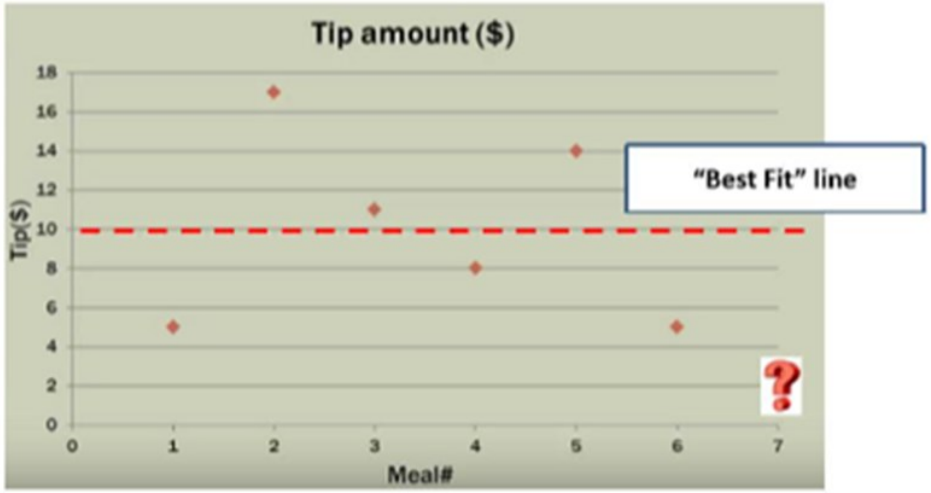
Gradient Descent Approach

How to choose θ_i's ?

Notion of Cost Function

Meal #	Tip amount ($)
1	5.00
2	17.00
3	11.00
4	8.00
5	14.00
6	5.00

mean = $10

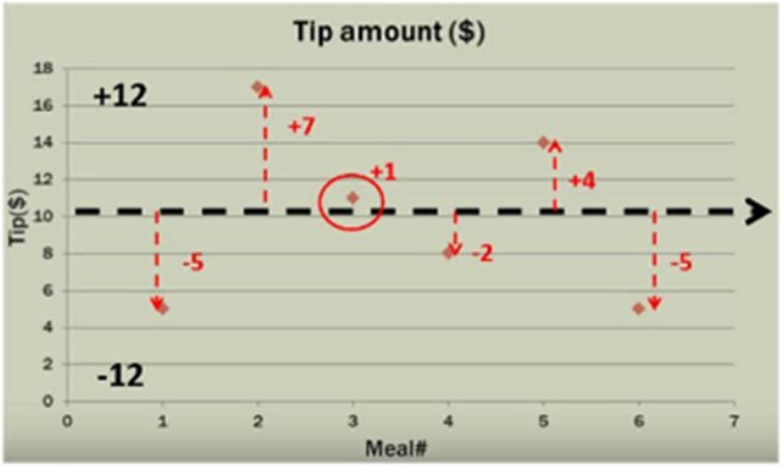


$y = \theta_0$

Notion of Cost Function

Meal #	Tip amount ($)
1	5.00
2	17.00
3	11.00
4	8.00
5	14.00
6	5.00

mean = $10



RESIDULAS (error): Distance from best fit line and the actual values

Meal#	Residual	Residual^2
1	−5	25
2	+7	49
3	+1	1
4	−2	4
5	+4	16
6	−5	25

Sum of Squared Errors (SSE) = 120

Notion of Cost Function

Meal #	Tip amount ($)
1	5.00
2	17.00
3	11.00
4	8.00
5	14.00
6	5.00

mean = $10

Meal	Total bill ($)	Tip amount ($)	$\hat{y}_i = 0.1462x - 0.8188$	$\hat{y}_i$ (predicted tip amount)
	x	y		
1	34	5	$\hat{y}_i = 0.1462(34) - 0.8188$	4.1505
2	108	17	$\hat{y}_i = 0.1462(108) - 0.8188$	14.9693
3	64	11	$\hat{y}_i = 0.1462(64) - 0.8188$	8.5365
4	88	8	$\hat{y}_i = 0.1462(88) - 0.8188$	12.0453
5	99	14	$\hat{y}_i = 0.1462(99) - 0.8188$	13.6535
6	51	5	$\hat{y}_i = 0.1462(51) - 0.8188$	6.6359
	$\bar{x} = 74$	$\bar{y} = 10$	Observed vs. Predicted	

$y = \theta_0 + \theta_1 x$

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}(\hat{y}^{(i)} - y^{(i)})^2$$

$$J(\theta) = \frac{1}{2n}\sum_{i=1}^{n}(h_\theta(x^{(i)}) - y^{(i)})^2$$

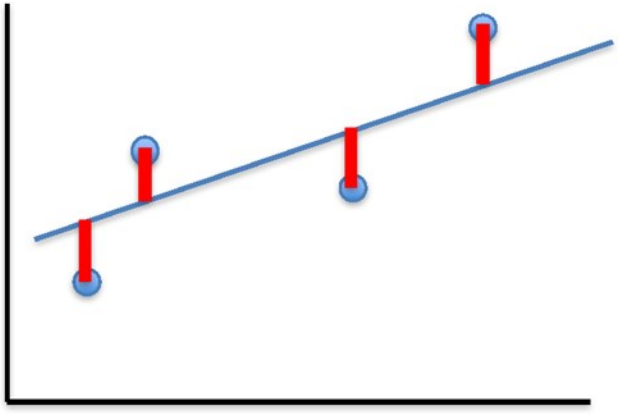
Linear Regression : Least Squares

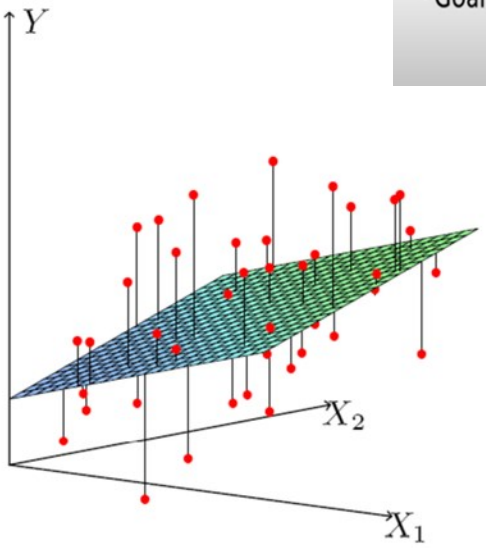
- Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Hypothesis $h_\theta(x) = \theta_0 + \theta_1 x$
- Parameters θ_0 and θ_1
- Cost Function $J(\theta_0,\theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^i) - y^{(i)})^2$
- Goal $\underset{\theta_0,\theta_1}{\text{minimize}}\ J(\theta_0,\theta_1)$





Intuition Behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

Source Credit : Based on example by Andrew Ng

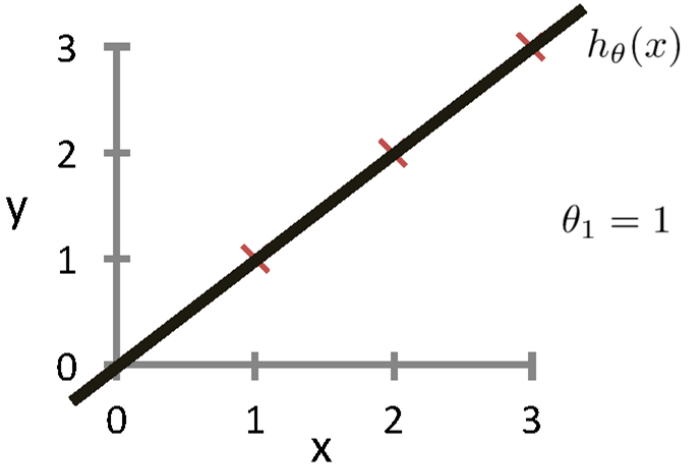
Intuition Behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

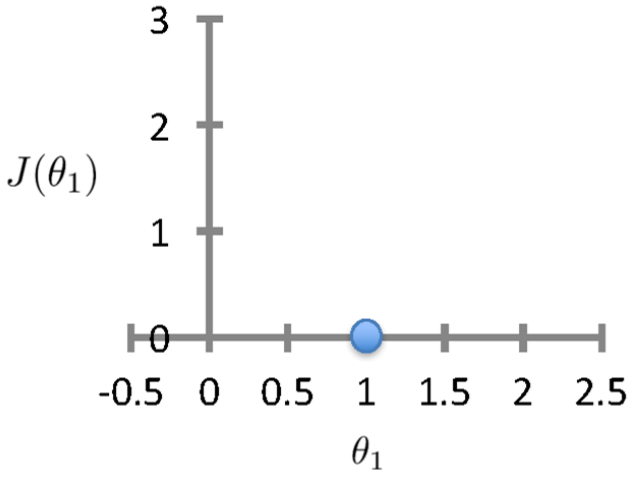
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)



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Intuition Behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

$h_\theta(x)$

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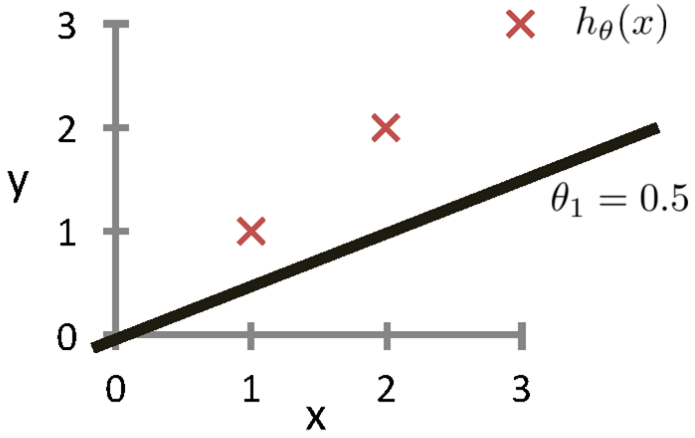
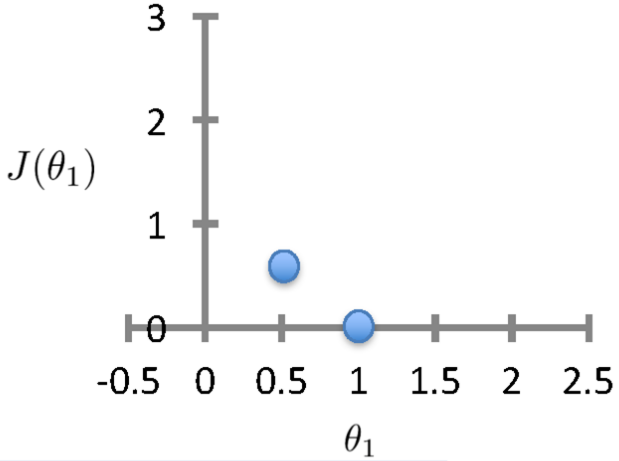


$J(\theta_1)$

(function of the parameter θ_1)



Based on example by Andrew Ng

$$J([0, 0.5]) = \frac{1}{2 \times 3}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right] \approx 0.58$$

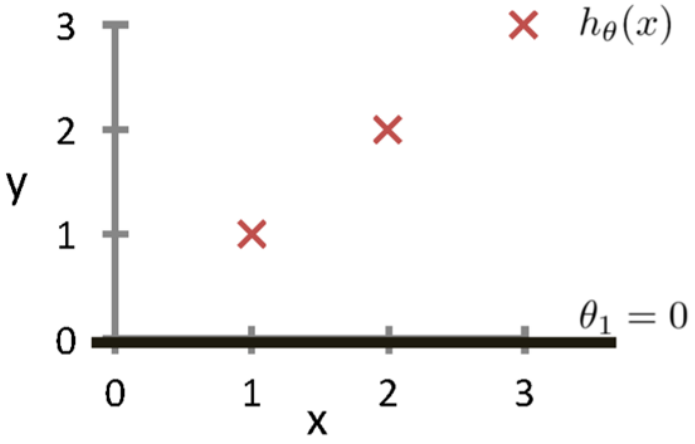
Intuition Behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

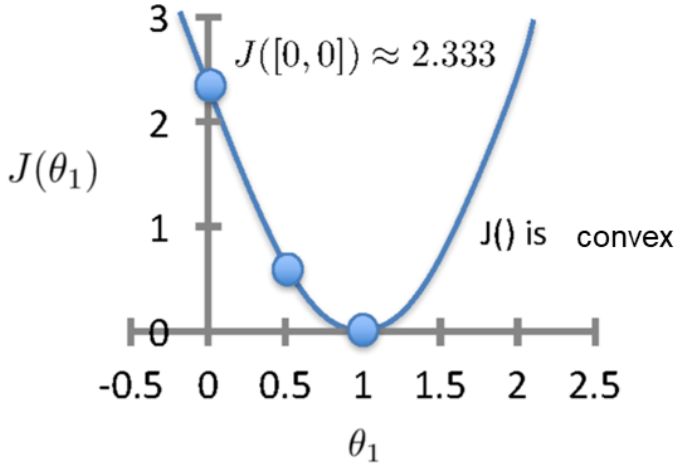
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)

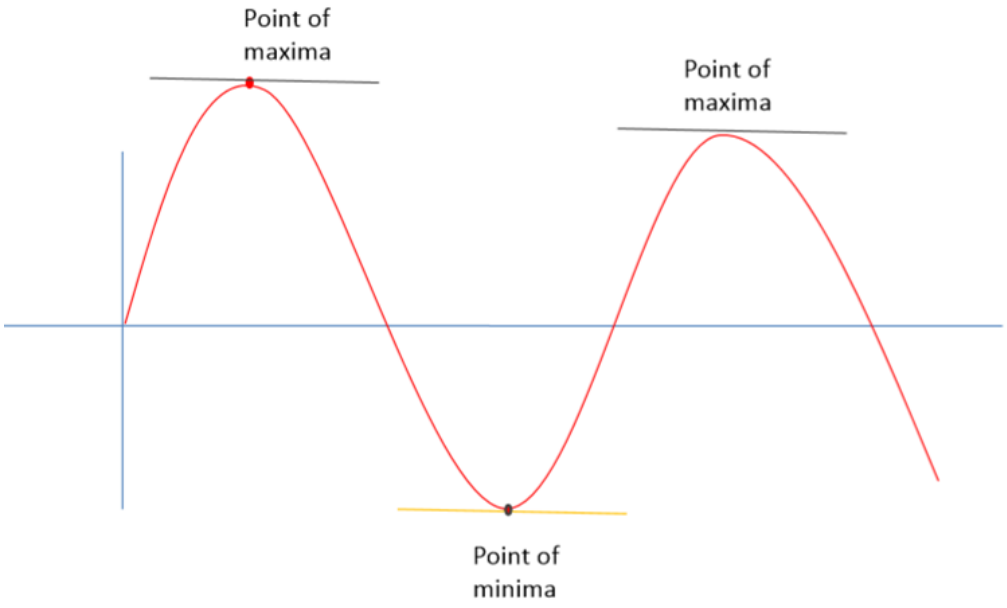


Source Credit : Based on example by Andrew Ng

Notion of Maxima and Minima of a function

In General

- For maxima and minima $m=dy/dx=\tan 0^0=0$
- $dy/dx = 0$ means tangent is parralel to X –axis.



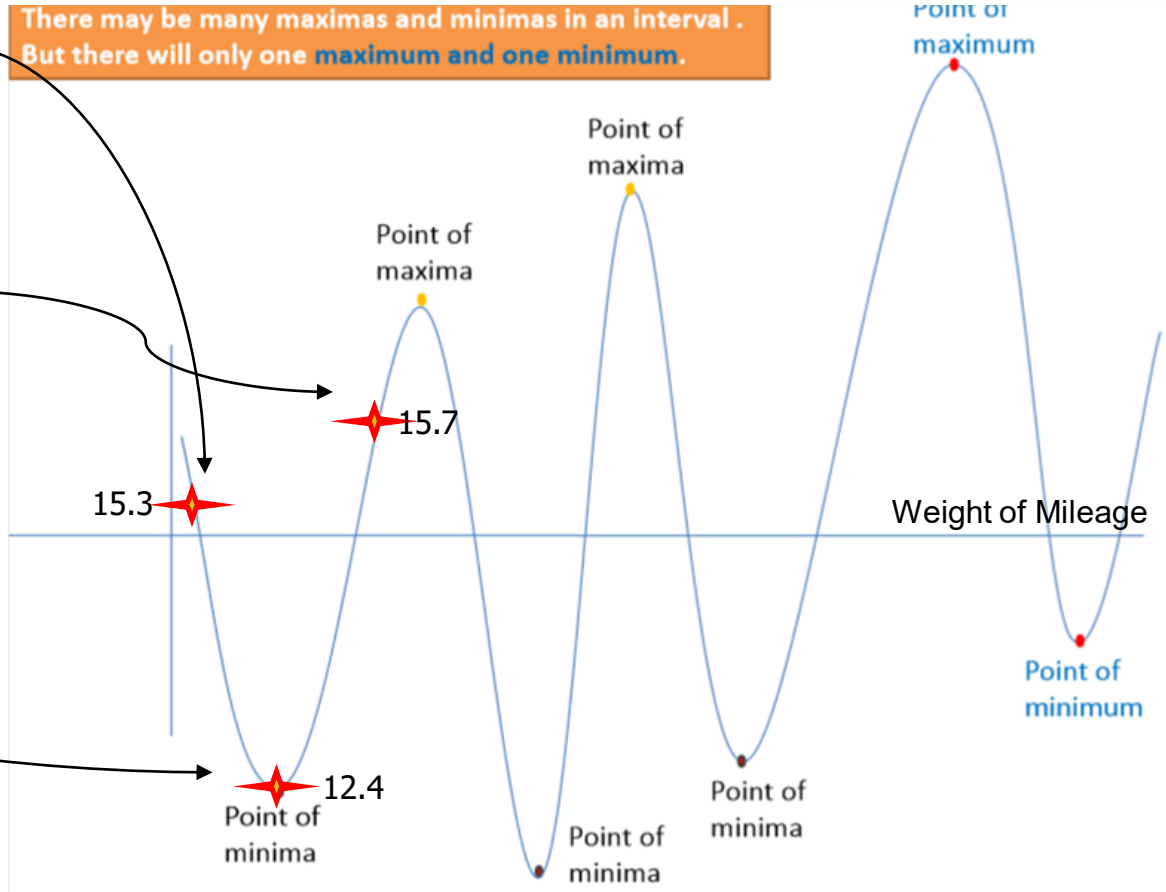
Notion of Maxima and Minima of a function

In Machine Learning

CarPrice = 1 + 0.05Mileage

CarPrice = 1 + 0.25Mileage

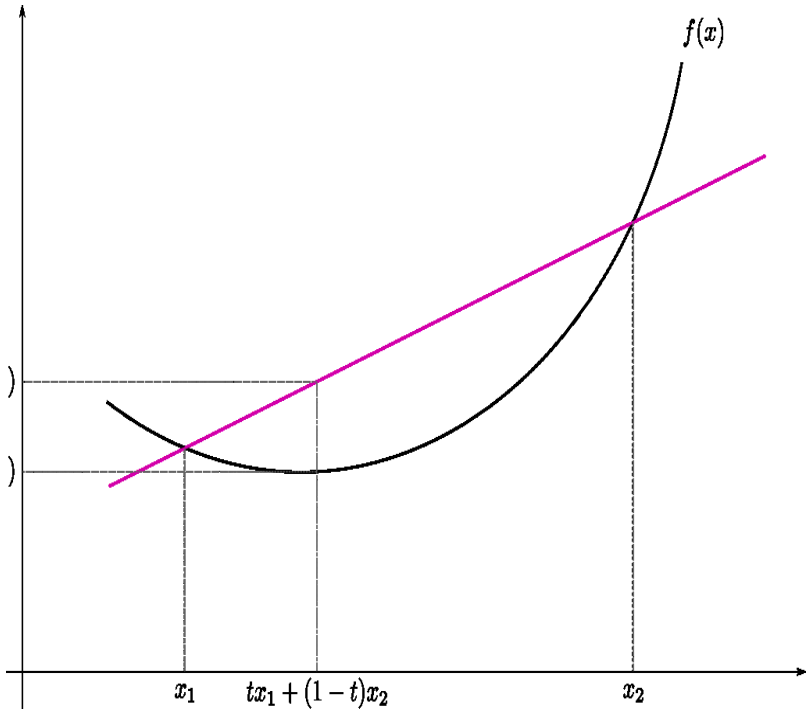
CarPrice = 1 + 0.75Mileage

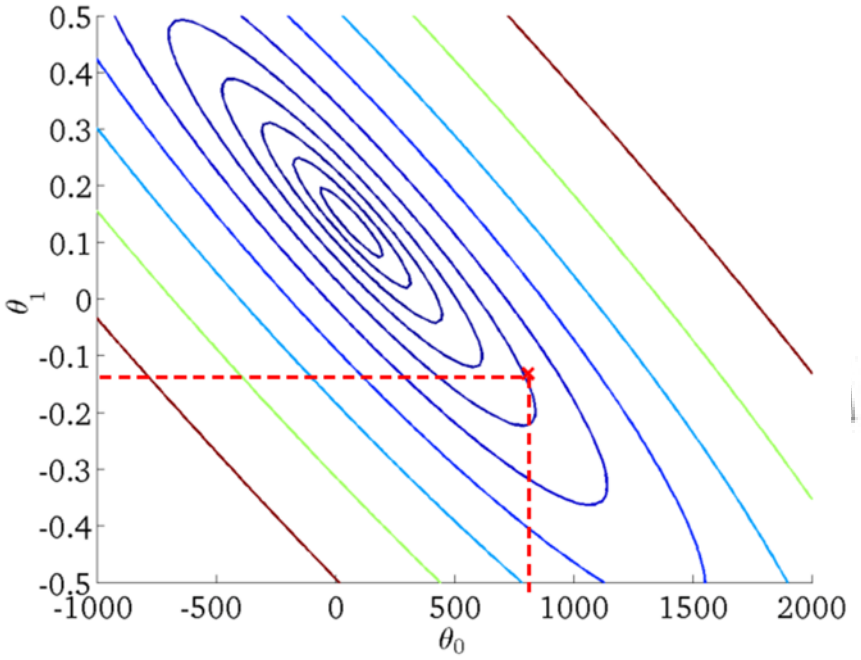


Mileage (in kmpl)	*Car Price (in cr)*
9.8	10.48
9.12	1.75
9.5	6.95
10	2.51

Sum of absolute Error / Training Error

Convex Function : Multivariate View





Real-valued function defined on an *n*-dimensional interval is called **convex** if the line segment between any two points on the graph of the function lies above or on the graph

Closed Form Solution

Vectorization

X No.of.Years of Experience (in Years)	Y Salary Of the Employee (in Lakhs)
1	2
2	3
3	4
4	5
5	6

- Benefits of vectorization
  - More compact equations
  - Faster code (using optimized matrix libraries)
- Consider our model:

$$h(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j$$

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \qquad \boldsymbol{x}^\mathsf{T} = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}$$

- Can write the model in vectorized form as $h(\boldsymbol{x}) = \boldsymbol{\theta}^\mathsf{T}\boldsymbol{x}$

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \quad \boldsymbol{x}^T = \begin{bmatrix} 1 & \textit{No.of.Years Experience} \end{bmatrix}$$

Vectorization

X No.of.Years of Experience (in Years)	Y Salary Of the Employee (in Lakhs)
1	2
2	3
3	4
4	5
5	6

- Consider our model for n instances:

$$h\left(\boldsymbol{x}^{(i)}\right) = \sum_{j=0}^{d} \theta_j x_j^{(i)}$$

- Let

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix}$$

Let:

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

$\boldsymbol{\theta} \in \mathbb{R}^{(d+1)\times 1}$ $\quad \boldsymbol{X} \in \mathbb{R}^{n\times(d+1)}$

- Can write the model in vectorized form as $h_{\boldsymbol{\theta}}$

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \quad \boldsymbol{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \end{bmatrix} \quad \boldsymbol{y} = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

Vectorization

X No.of.Years of Experience (in Years)	Y Salary Of the Employee (in Lakhs)
1	2
2	3
3	4
4	5
5	6

- For the linear regression cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

$$= \frac{1}{2n}\sum_{i=1}^{n}\left(\boldsymbol{\theta}^{\intercal}\boldsymbol{x}^{(i)} - y^{(i)}\right)^2$$

$$= \frac{1}{2n}\underbrace{(\boldsymbol{X\theta} - \boldsymbol{y})^{\intercal}}_{\mathbb{R}^{1\times n}}\underbrace{(\boldsymbol{X\theta} - \boldsymbol{y})}_{\mathbb{R}^{n\times 1}}$$

$\mathbb{R}^{n\times(d+1)}$, $\mathbb{R}^{(d+1)\times 1}$

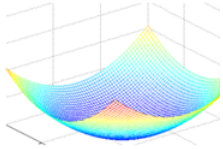
Let:

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

$$\boldsymbol{\theta}^{T} = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \quad \boldsymbol{X} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} \quad \boldsymbol{y} = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

Vectorization

- Instead of using GD, solve for optimal θ analytically
  - Notice that the solution is when $\frac{\partial}{\partial \theta} J(\theta) = 0$



- Derivation:

$$\mathcal{J}(\theta) = \frac{1}{2n}(X\theta - y)^T(X\theta - y)$$

1 x 1

$$\propto \theta^T X^T X\theta - \boxed{y^T X\theta} - \boxed{\theta^T X^T y} + y^T y$$

$$\propto \theta^T X^T X\theta - 2\theta^T X^T y + y^T y$$

Take derivative and set equal to 0, then solve for θ:

$$\frac{\partial}{\partial \theta}(\theta^T X^T X\theta - 2\theta^T X^T y + \cancel{y^T y}) = 0$$

$$(X^T X)\theta - X^T y = 0$$

$$(X^T X)\theta = X^T y$$

Closed Form Solution: $\theta = (X^T X)^{-1} X^T y$

Vectorization

- Can obtain θ by simply plugging X and y into

$$\theta = (X^T X)^{-1} X^T y$$

$$X = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(i)} & \dots & x_d^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_d^{(n)} \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

- If $X^T X$ is not invertible (i.e., singular), may need to:
  - Use pseudo-inverse instead of the inverse
    - In python, `numpy.linalg.pinv(a)`
  - Remove redundant (not linearly independent) features
  - Remove extra features to ensure that $d \leq n$

Fit the Linear Regression Model :

Using Closed Form – Problem Type 1

X No.of.Years of Experience (in Years)	Y Salary Of the Employee (in Lakhs)
1	2
2	3
3	4
4	5
5	6

$$\left(X^T \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} * X \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \end{bmatrix} \right) -1 * X^T \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} * y \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

$$\left(\begin{bmatrix} 5 & 15 \\ 15 & 55 \end{bmatrix} \right) -1 * X^T \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} * y \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

$$\left(\begin{bmatrix} 1.1 & -0.3 \\ -0.3 & 0.1 \end{bmatrix} \right) * X^T \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} * y \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

Can obtain θ by simply plugging X and y into

$$\theta = (X^\intercal X)^{-1} X^\intercal y$$

$$\begin{bmatrix} 0.8 & 0.5 & 0.2 & -0.1 & -0.4 \\ -0.2 & -0.1 & 0 & 0.1 & -0.2 \end{bmatrix} * y \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

$$\theta^T = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \quad X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix} \quad y = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{bmatrix}$$

$$\theta = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Gradient Descent Approach

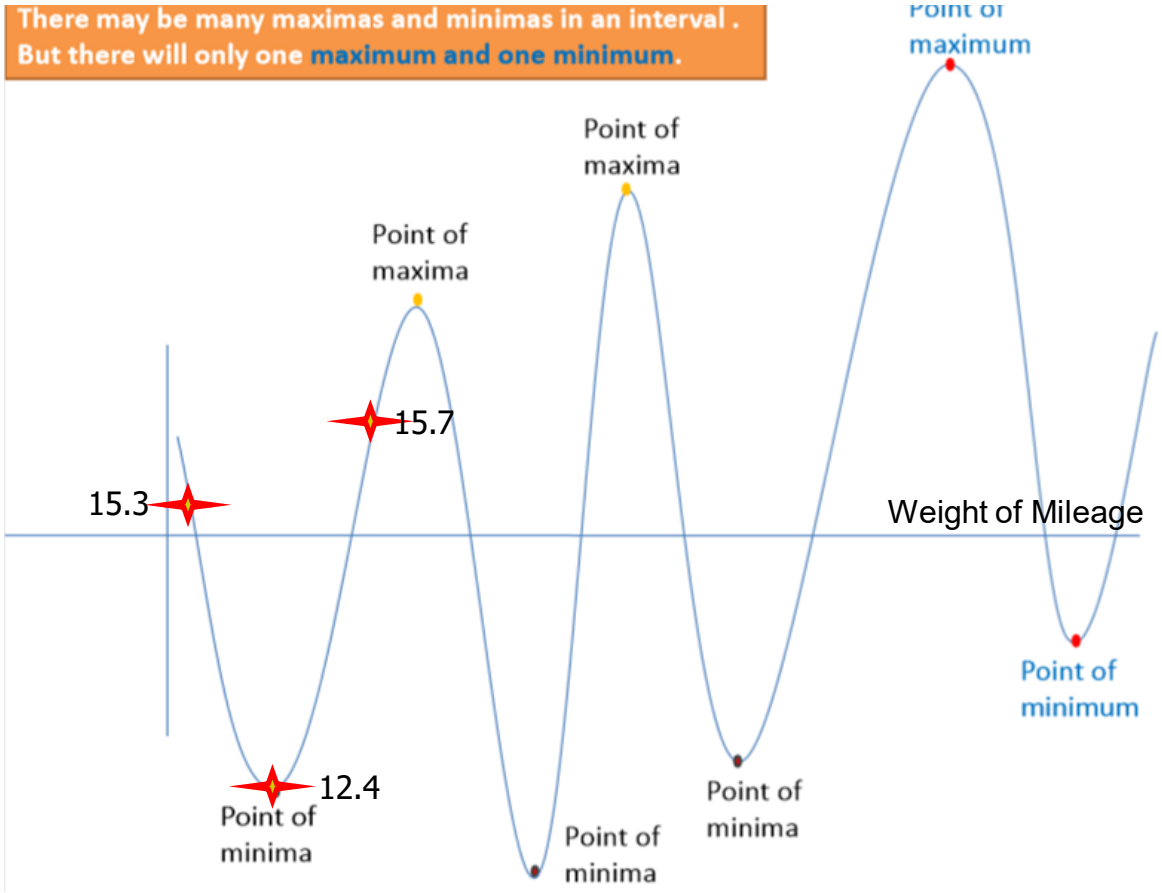
BITS Pilani

Notion of Gradient Descent

CarPrice = 1 + 0.05Mileage

CarPrice = 1 + 0.25Mileage

CarPrice = 1 + 0.75Mileage



Mileage (in kmpl)	*Car Price (in cr)*
9.8	10.48
9.12	1.75
9.5	6.95
10	2.51

Sum of absolute Error / Training Error

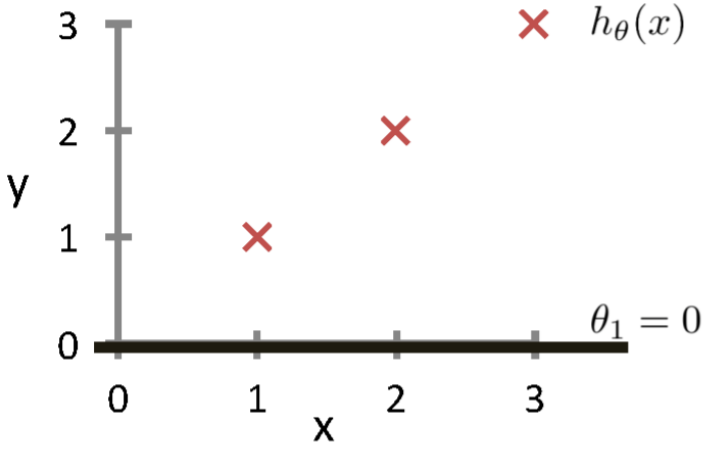
Intuition Behind Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

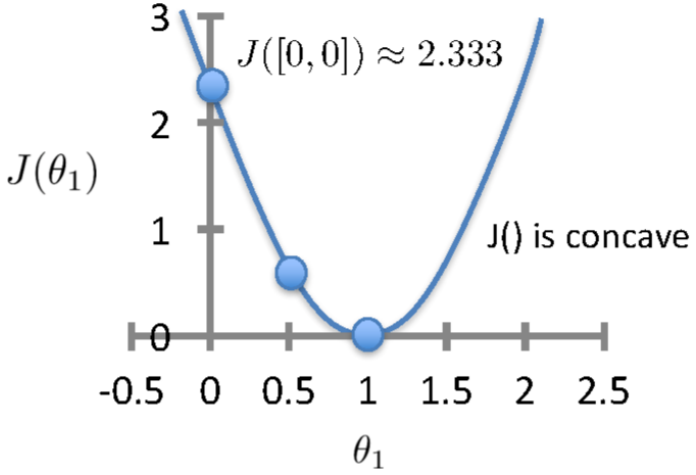
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



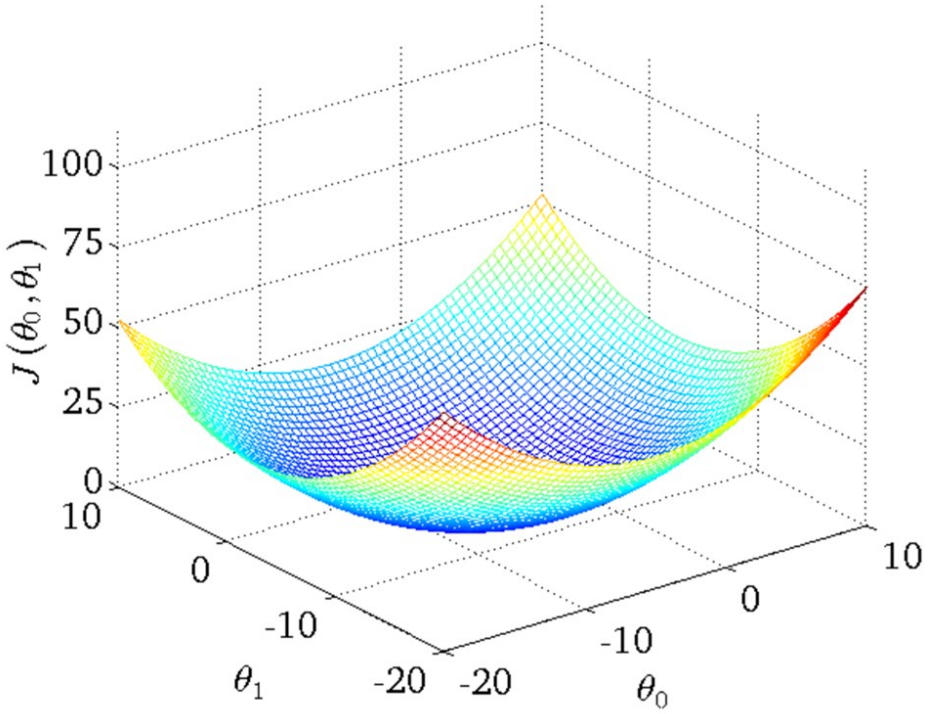
$J(\theta_1)$

(function of the parameter θ_1)



Source Credit : Based on example by Andrew Ng

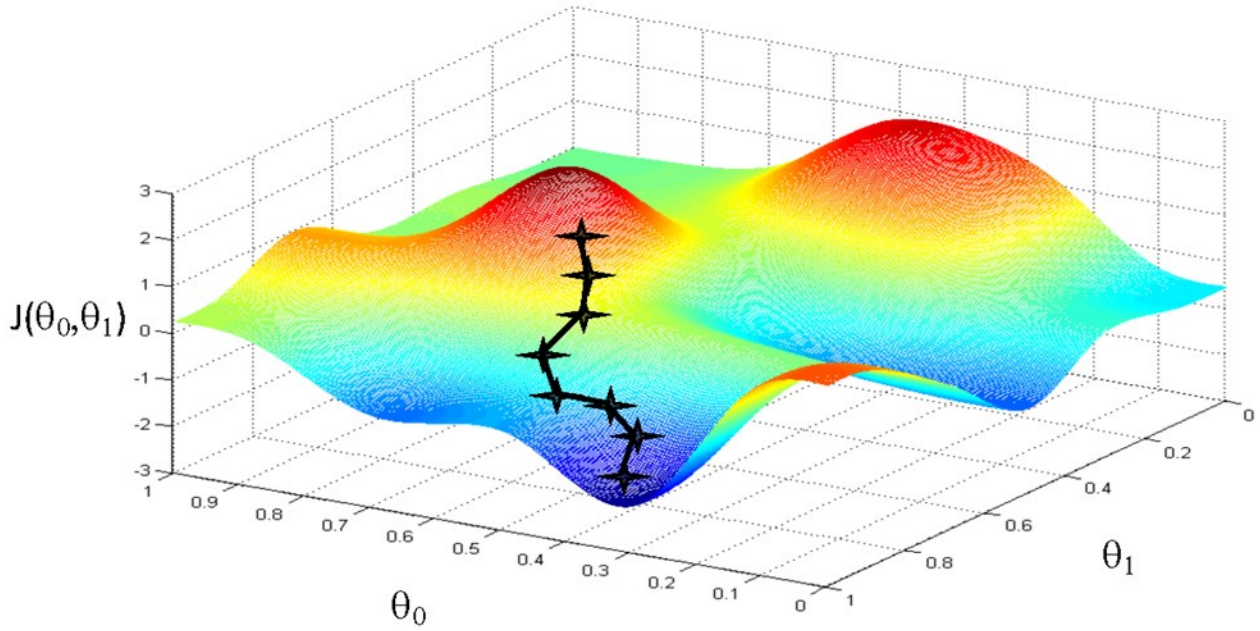
Intuition Behind Cost Function



Source Credit : Based on example by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for θ to reduce $J(\theta)$



Source Credit : Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
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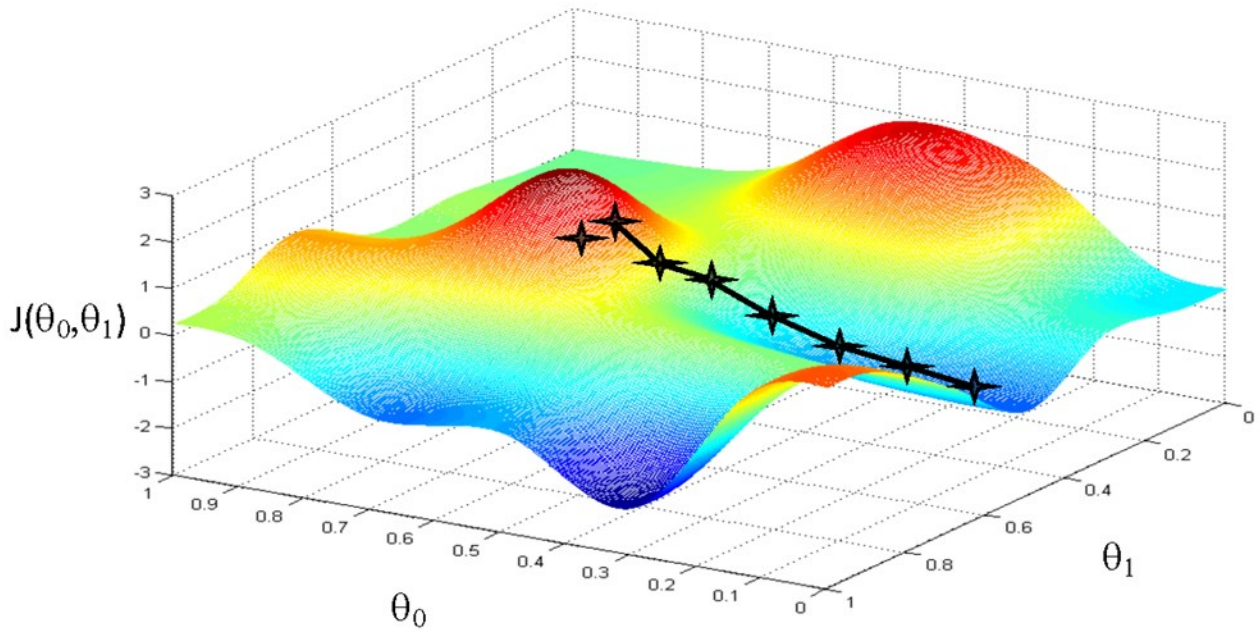
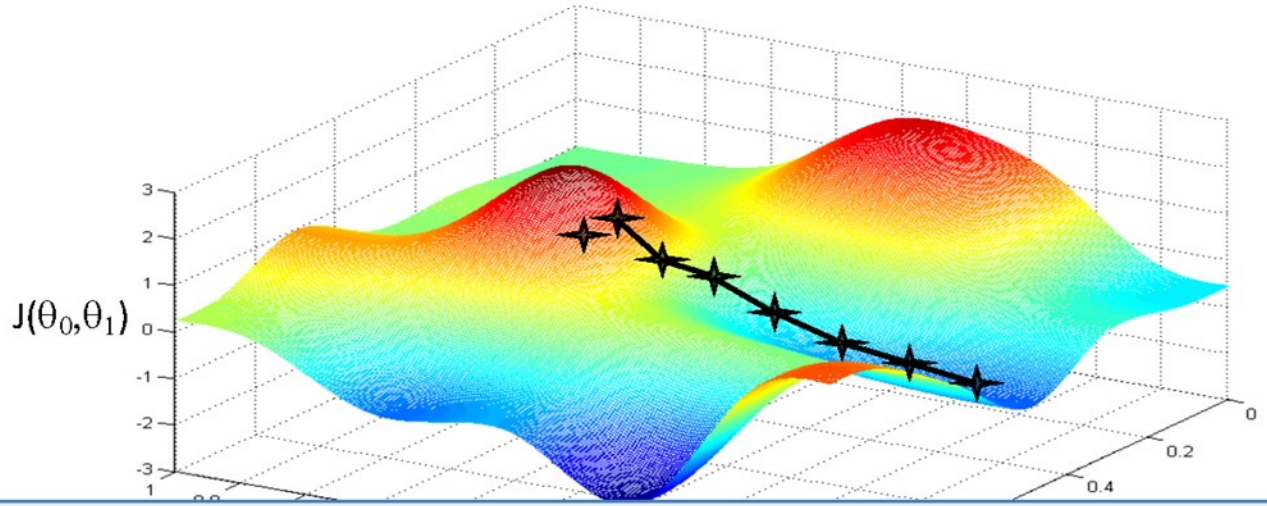


Source Credit : Figure by Andrew Ng

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for θ to reduce $J(\theta)$



Since the least squares objective function is convex (concave), we don't need to worry about local minima

Source Credit : Figure by Andrew Ng

Gradient Descent

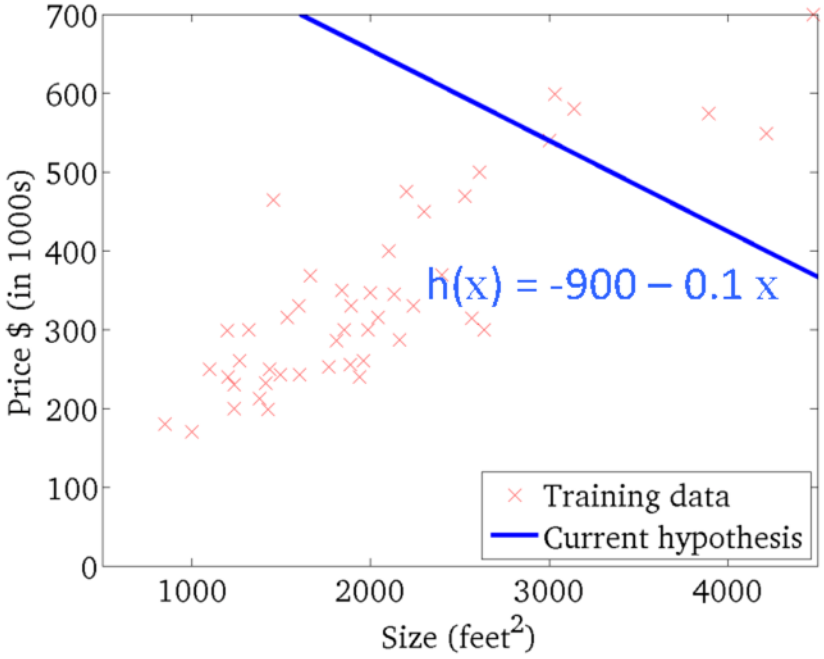
Size in feet² (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
…	…

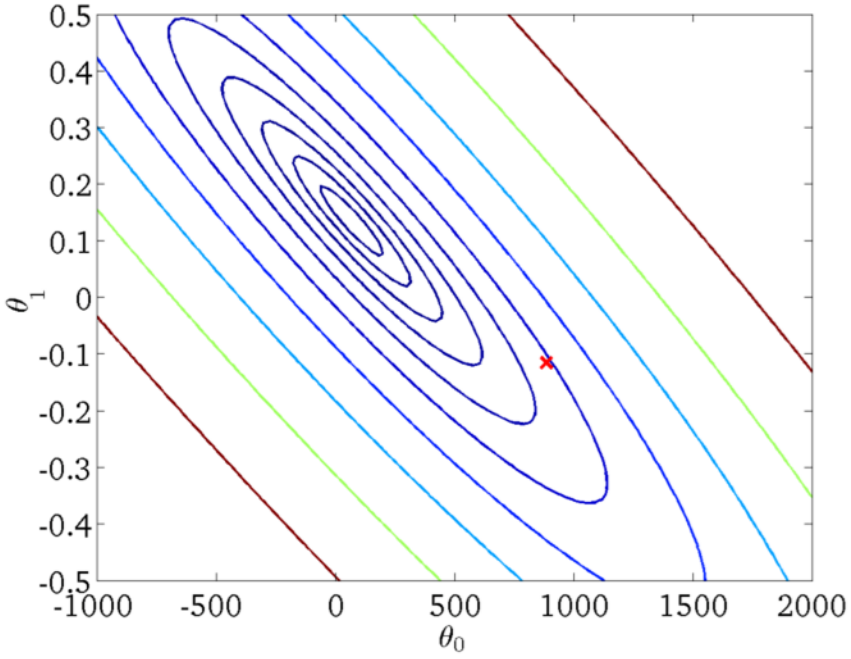
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)

$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



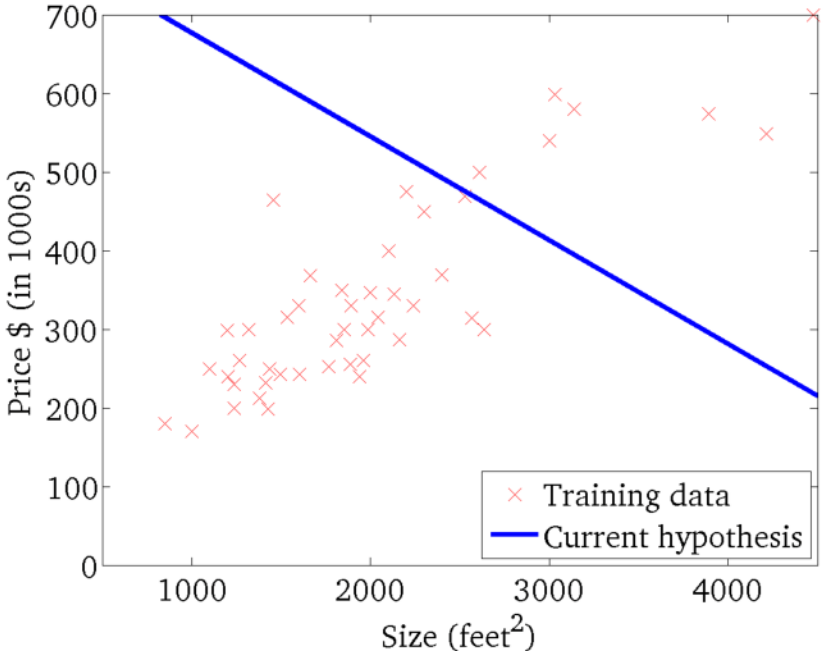


Source Credit : Slide by Andrew Ng

Gradient Descent

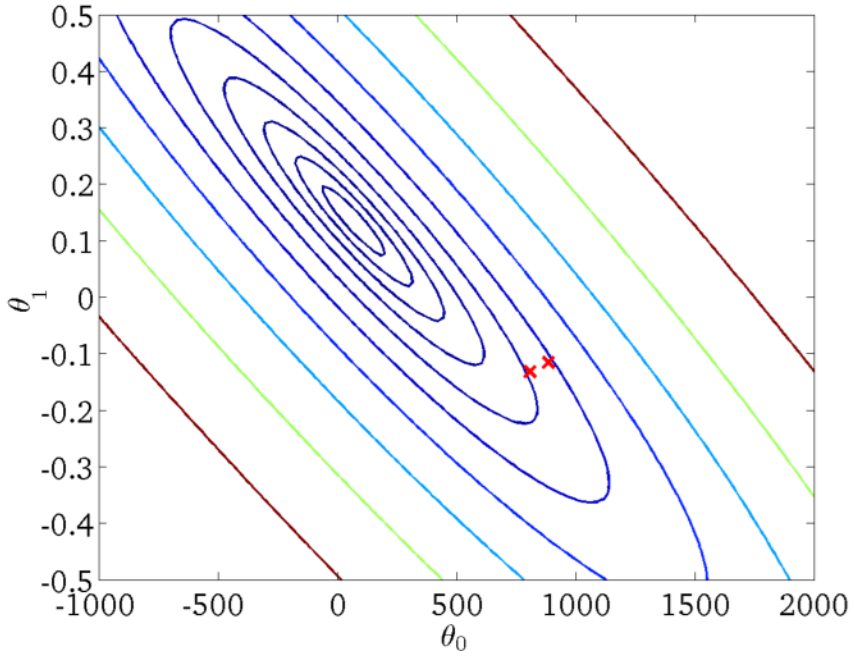
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

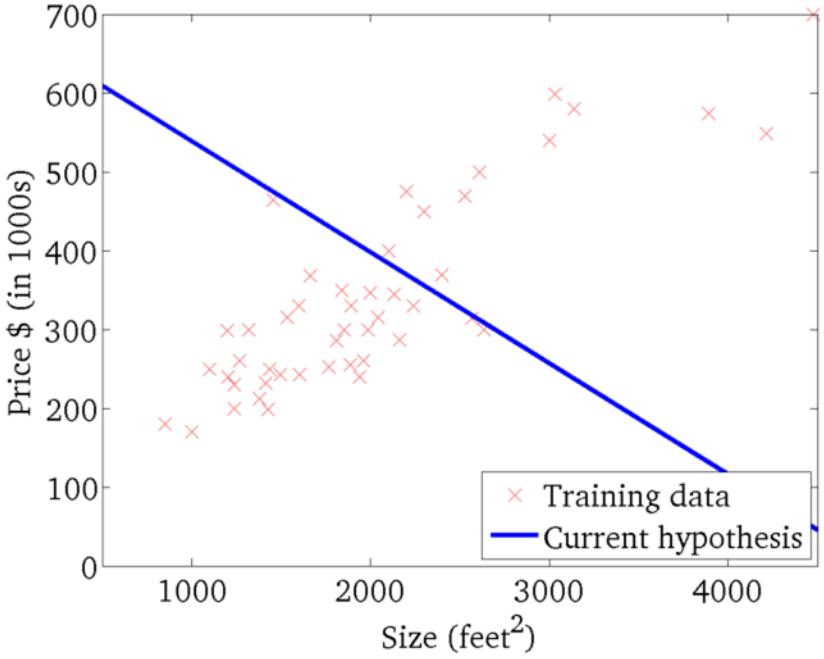


Source Credit : Slide by Andrew Ng

Gradient Descent

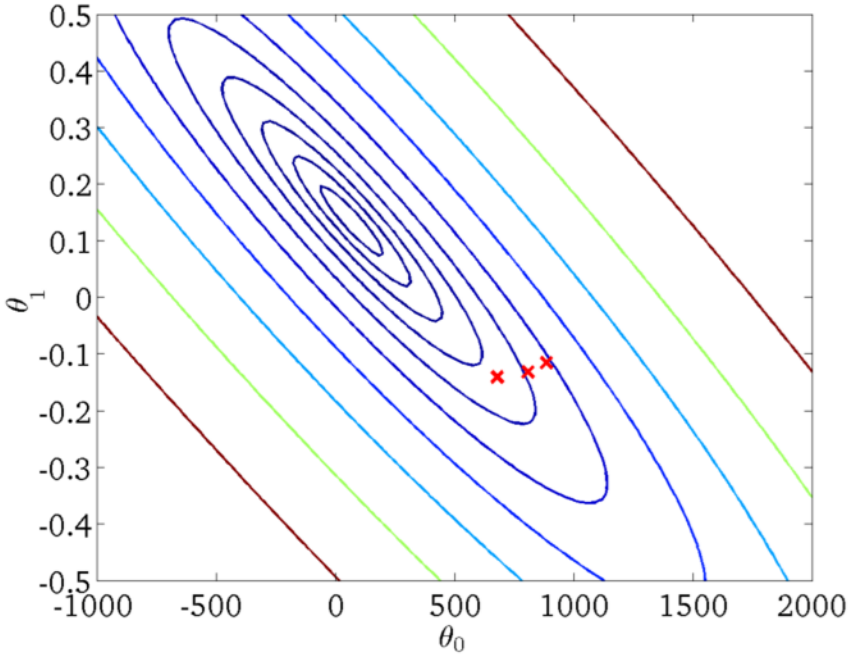
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

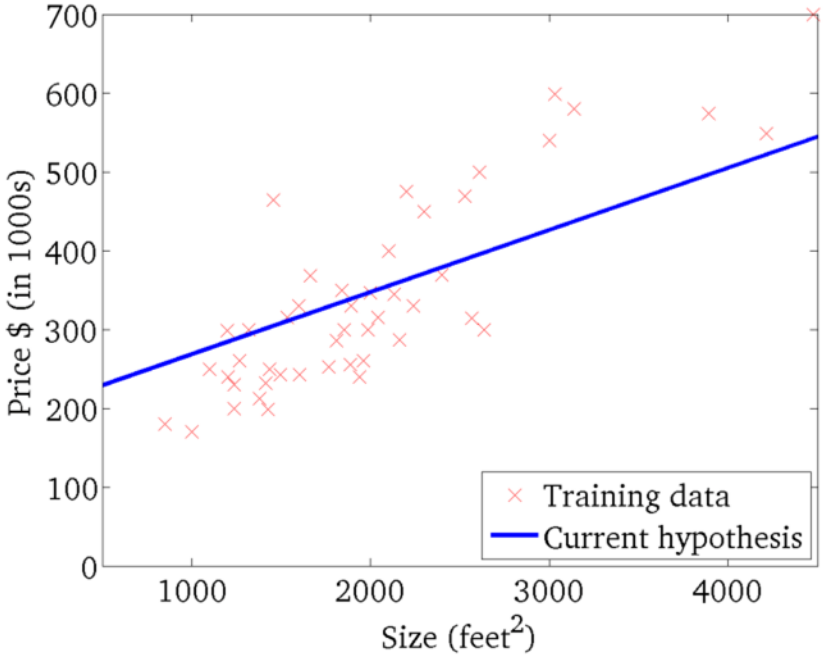


Source Credit : Slide by Andrew Ng

Gradient Descent
(….After Few Iteration or SEARCH!!)

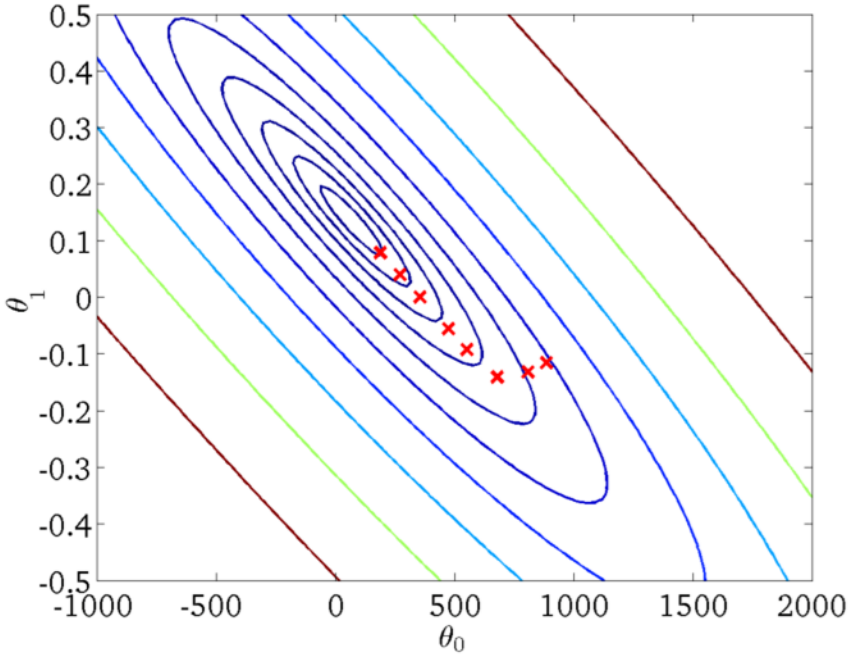
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

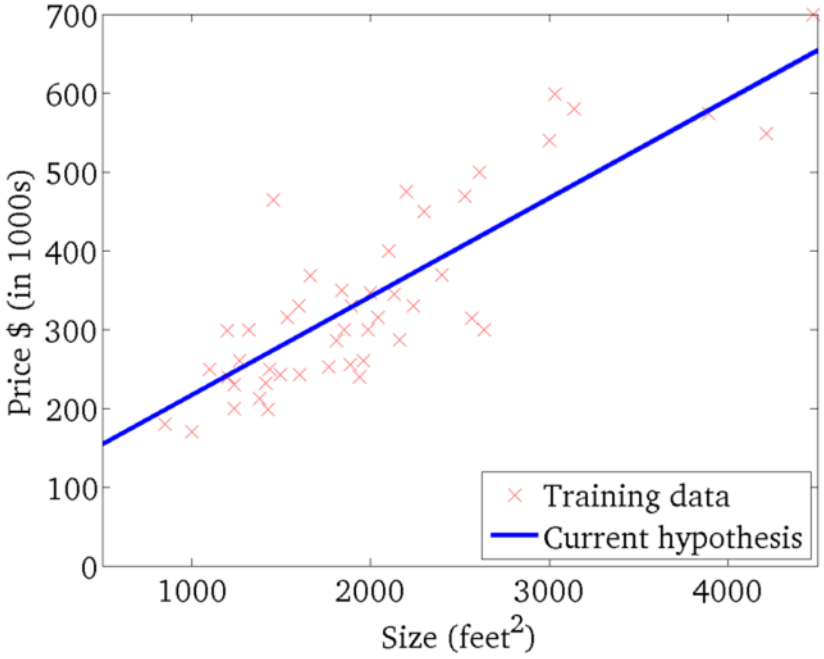


Source Credit : Slide by Andrew Ng

Gradient Descent

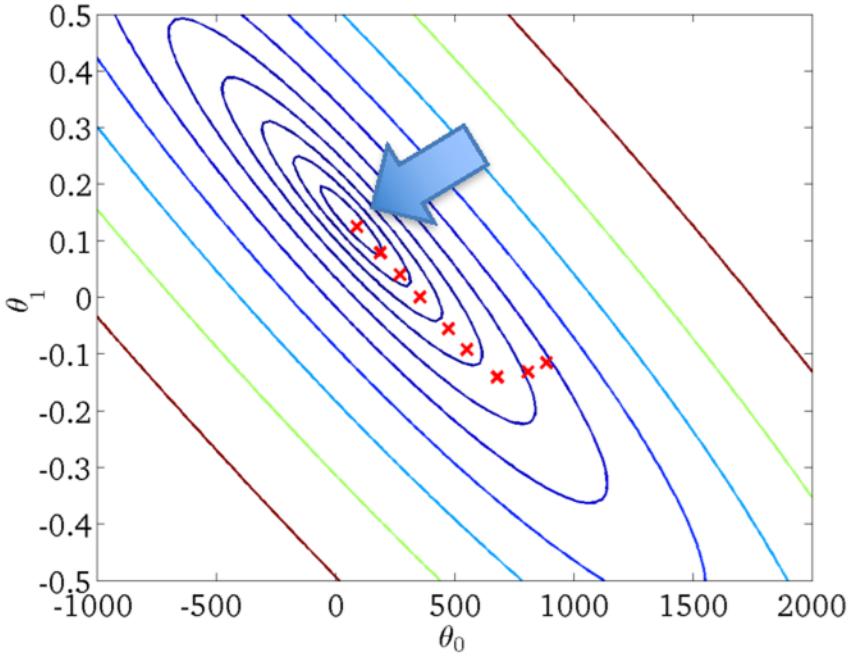
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



Source Credit : Slide by Andrew Ng

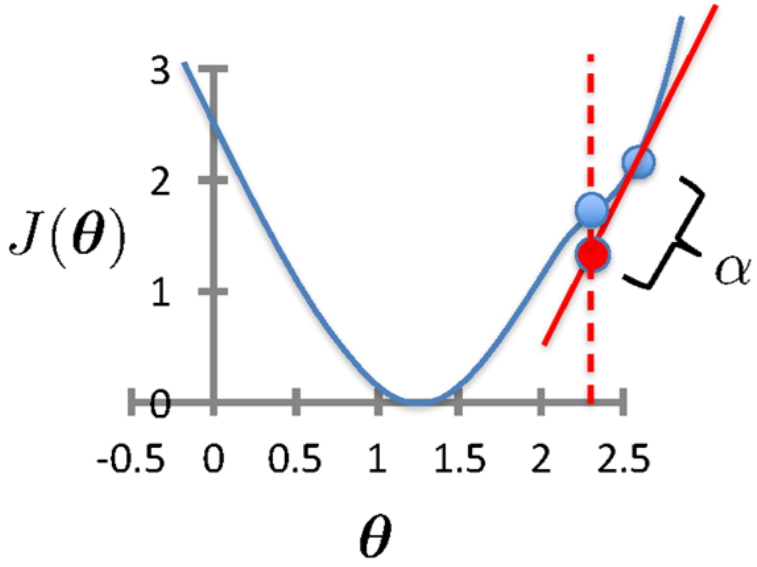
Gradient Descent

- Initialize θ
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

For Linear Regression:

$$\frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta}) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2$$

$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) \times \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \right) x_j^{(i)}$$

Gradient Descent for Linear Regression

- Initialize θ
- Repeat until convergence

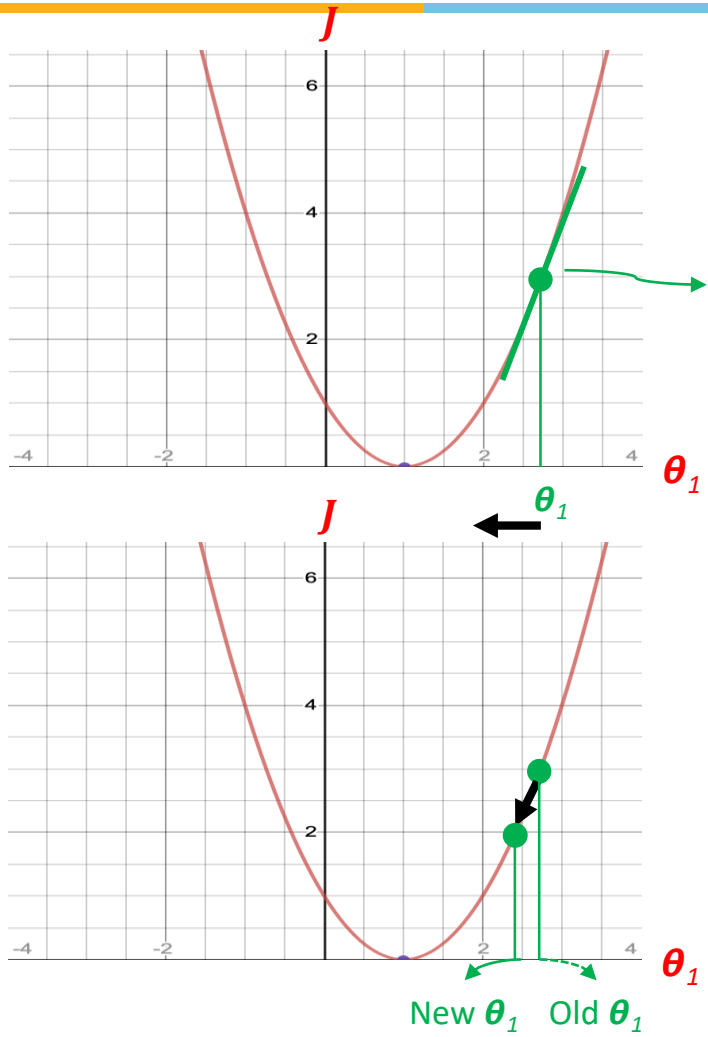
$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)}$$

simultaneous update for j = 0 ... d

- To achieve simultaneous update
  - At the start of each GD iteration, compute $h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right)$
  - Use this stored value in the update step loop
- Assume convergence when $\| \boldsymbol{\theta}_{new} - \boldsymbol{\theta}_{old} \|_2 < \epsilon$

L_2 norm: $\| \boldsymbol{v} \|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \ldots + v_{|v|}^2}$

Guarantee of Convergence



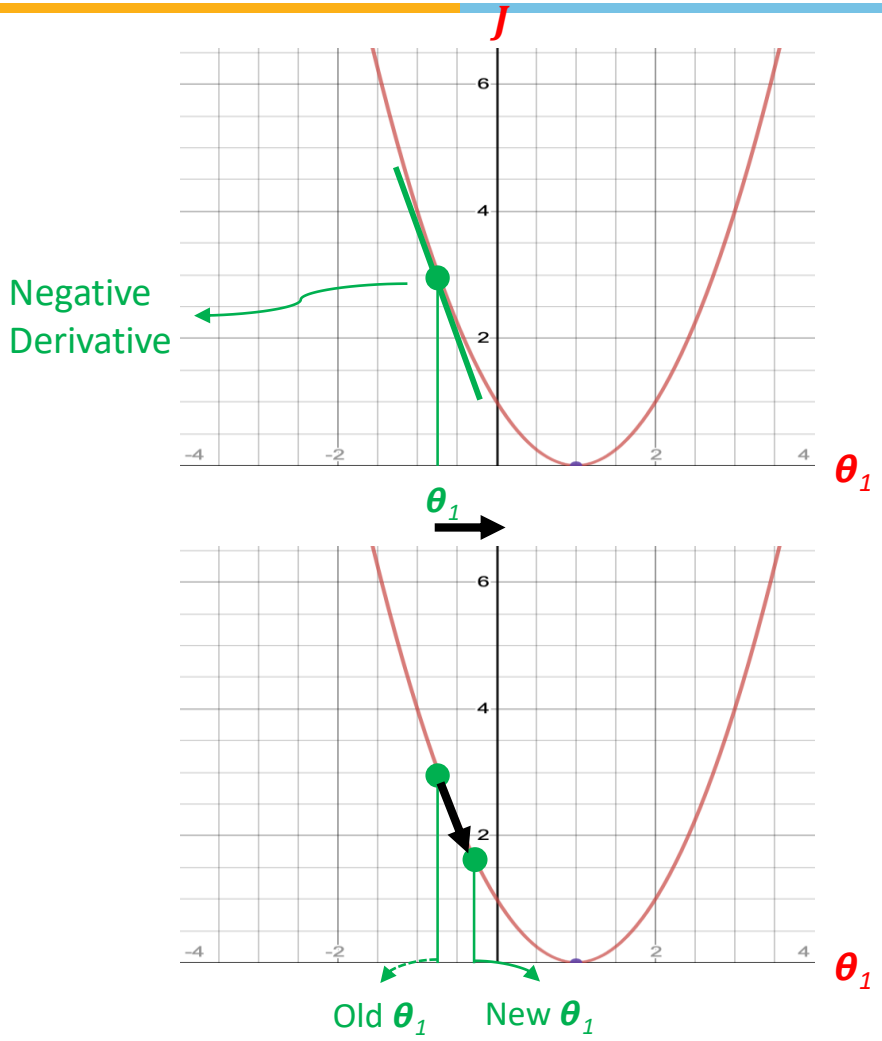
Source Credit: Prof. Mohammad Hammoud

$$\theta_1 = \theta_1 - \alpha \frac{d J(\theta_1)}{d \theta_j}$$

$$= \theta_1 - \alpha \, (Positive\ Number)$$

Decrease θ_1 by a certain value

Guarantee of Convergence



Source Credit: Prof. Mohammad Hammoud

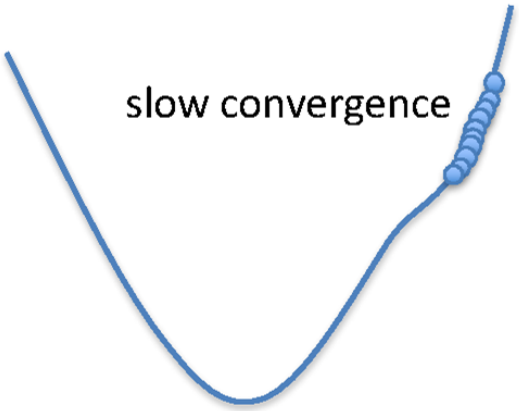
$$\theta_1 = \theta_1 - \alpha \frac{\boldsymbol{d}\, \boldsymbol{J(\theta_1)}}{\boldsymbol{d}\, \theta_j}$$

$$= \theta_1 - \alpha\, (Negative\ Number)$$

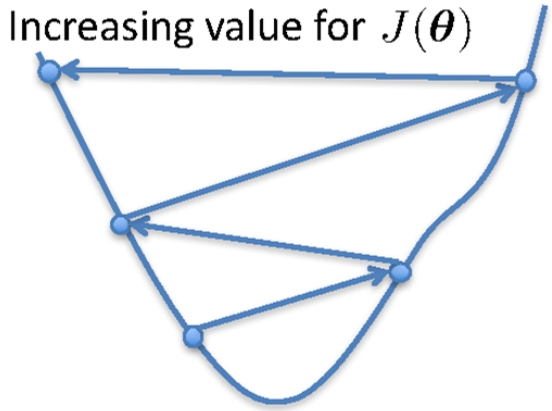
Increase θ_1 by a certain value

Choosing Learning Rate

α too small



α too large



- May overshoot the minimum
- May fail to converge
- May even diverge

To see if gradient descent is working, print out $J(\theta)$ each iteration

- The value should decrease at each iteration
- If it doesn't, adjust α

Gradient Descent algorithm : Effect of Feature Scaling

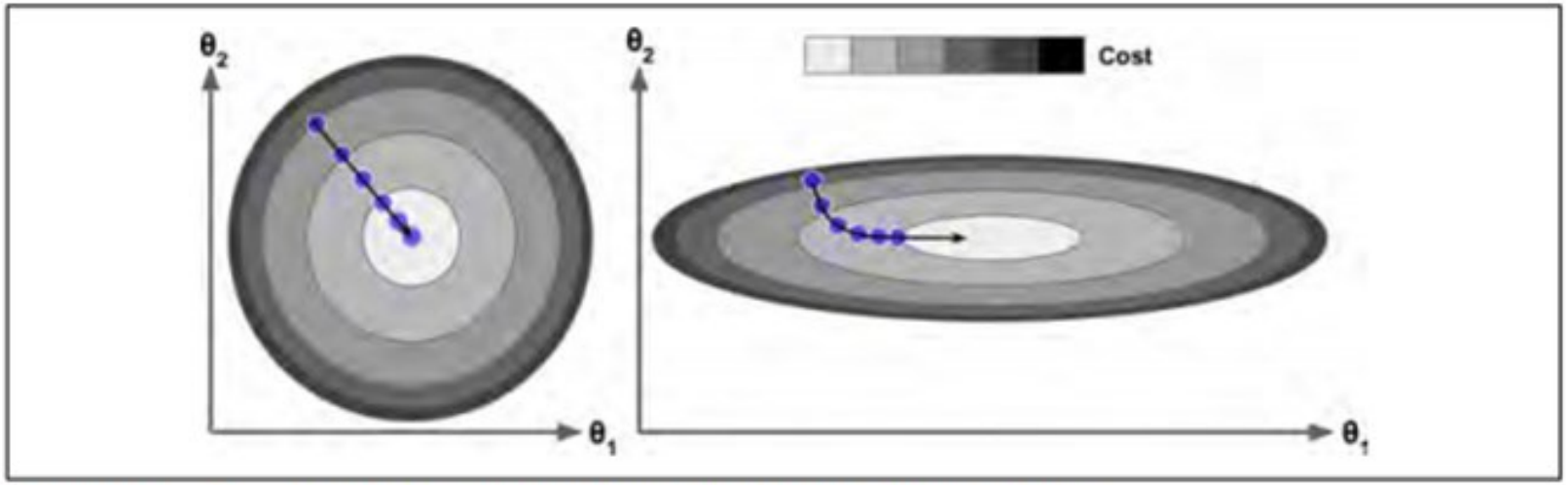


Figure 4-7. Gradient Descent with and without feature scaling

Gradient Descent algorithm : Effect of Learning Rate :

Problem Type 2 – Interpretation of Convergence or Effect of Hyper parameters

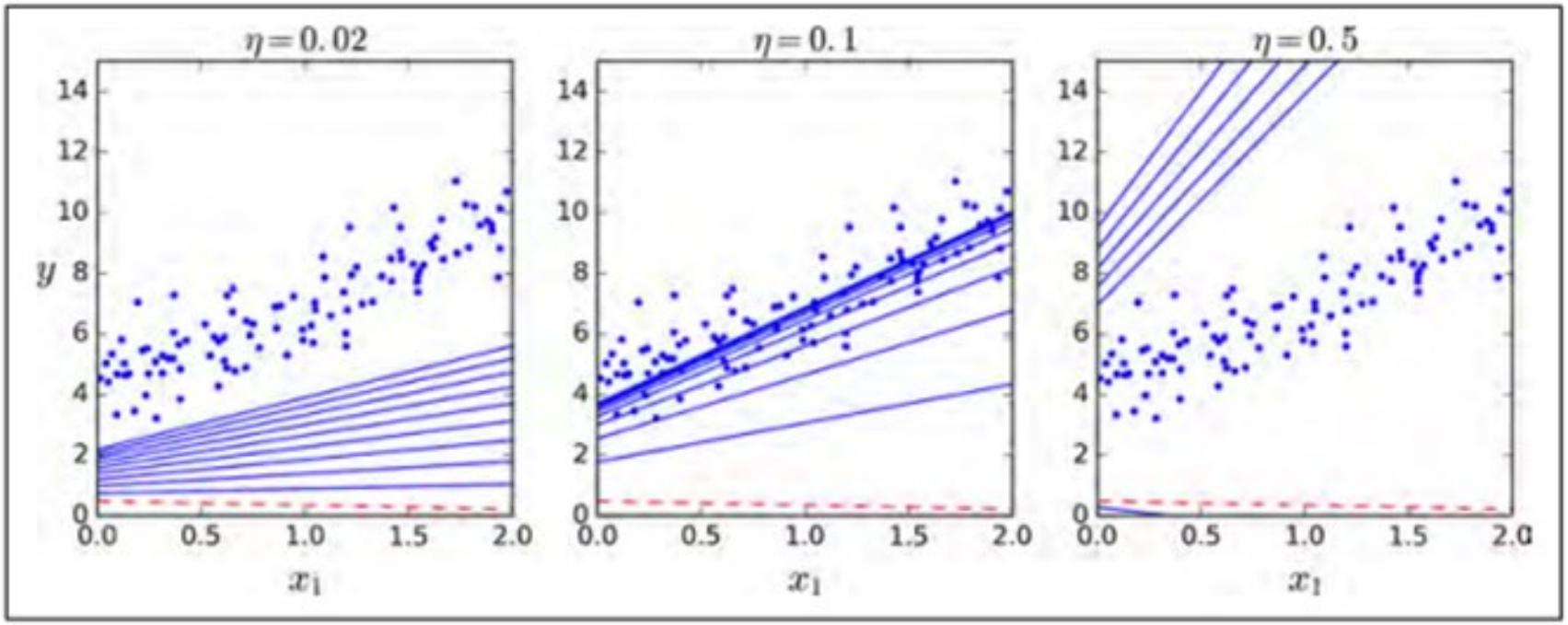


Figure 4-8. Gradient Descent with various learning rates

Fit a linear Regression Line :

Gradient Descent : Problem Type 3

Steps :

(Assuming : 'n' no.of.instances and two predictors {x1, x2} and linear regression)

1. Identification of the equations y = w0+w1X1+W2X2
2. Cost function & derivative
    1. W0` = w0 – 1/n * learning rate * (sum (w0+w1X1+W2X2 - y))
    2. W1` = w1 – 1/n * learning rate * (sum (w0+w1X1+W2X2 - y) * x1)
    3. W2` = w2 – 1/n * learning rate * (sum (w0+w1X1+W2X2 - y)*x2)
3. Apply the equations

Fit a linear Regression Line :

Gradient Descent

Fit a linear regression. Show only the first iteration of Gradient descent algorithm using learning rate of **0.02** for the following data , if the Relative Risk of Coronary Heart Disease is believed to be only linearly dependent on BMI as well as Diastolic Pressure. Assume the intercept of the regression model as **5** and the slope of independent variables as **-0.03 (negative)**.

Patient	Systolic Pressure mm Hg	Diastolic Pressure mm Hg	BMI	Waist Circumference Threshold cm	RR-CHD (Relative Risk of Coronary Heart Disease)
1	140	80	35	100	1.81
2	120	80	25	80	1.22
3	130	100	30	60	1.71

Steps :

1. Identification of the equations y = w0+w1X1+W2X2
2. Cost function & derivative
    1. W0` = w0 – 1/3 * learning rate * (sum (w0+w1X1+W2X2 - y))
    2. W1` = w1 – 1/3 * learning rate * (sum (w0+w1X1+W2X2 - y) * x1)
    3. W2` = w2 – 1/3 * learning rate * (sum (w0+w1X1+W2X2 - y)*x2)
3. Apply the equations

Fit a linear Regression Line :

Gradient Descent

Fit a linear regression. Show only the first iteration of Gradient descent algorithm using learning rate of **0.02** for the following data , if the Relative Risk of Coronary Heart Disease is believed to be only linearly dependent on BMI as well as Diastolic Pressure. Assume the intercept of the regression model as **5** and the slope of independent variables as **-0.03 (negative)**.

Patient	Systolic Pressure mm Hg	Diastolic Pressure mm Hg	BMI	Waist Circumference Threshold cm	RR-CHD (Relative Risk of Coronary Heart Disease)
1	140	80	35	100	1.81
2	120	80	25	80	1.22
3	130	100	30	60	1.71

Steps :

1. Identification of the equations: RR-CHD = 5 – 0.03 * BMI – 0.03 * DiastolicPressure
2. Cost function & derivative
   1. W0` = w0 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD))
      = 5 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD))
   2. W1` = w1 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD) * BMI)
      = -0.03 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD) * BMI)
   3. W2` = w2 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD) * DiastolicPresure)
      = -0.03 – 1/3 * 0.02 * (sum (5-0.03BMI-0.03DiastolicPresure - RRCHD) * DiastolicPresure)
3. Apply the equations : Answer at the end of first iteration:
   W0 = 5.0016 , W1 = 0.0476, w2= 0.179

Closed Form Solution Vs. Gradient Descent

Gradient Descent	Closed Form Solution
• Requires multiple iterations • Need to choose α • Works well when n is large • Can support incremental learning	• Non-iterative • No need for α • Slow if n is large – Computing $(X^T X)^{-1}$ is roughly $O(n^3)$

References

- T1 - Chapter 1 – Machine Learning, Tom Mitchell
- Chapter 1, 2 – Introduction to Machine Learning, 2nd edition, Ethem Alpaydin
- R1 – Chapter #1, # 3,#4 (Christopher M. Bhisop, Pattern Recognition & Machine Learning) & Refresh your MFDS course basics

Thank you !

Next Session Plan:

- Variants of Gradient Descent
- Frequent Evaluation Metrics for Linear Regression Models
- Notion of Linear Basis Functions
- Notion of Bias vs Variance
- Ways to Handle Overfitting
- Types of Regularization