CS1138

Machine Learning

Lecture : Gradient Descent

(Slide Credits: Andrew Ng)

Arpan Gupta

Have some function $J(\theta_0, \theta_1)$ $J(\theta_0, \theta_1, \theta_2, \ldots, \theta_n)$

Want $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$ $\min_{\theta_0, \ldots, \theta_n} J(\theta_0, \ldots, \theta_n)$

Outline:

- Start with some θ_0, θ_1 (say $\theta_0 = 0, \theta_1 = 0$)
- Keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$ until we hopefully end up at a minimum

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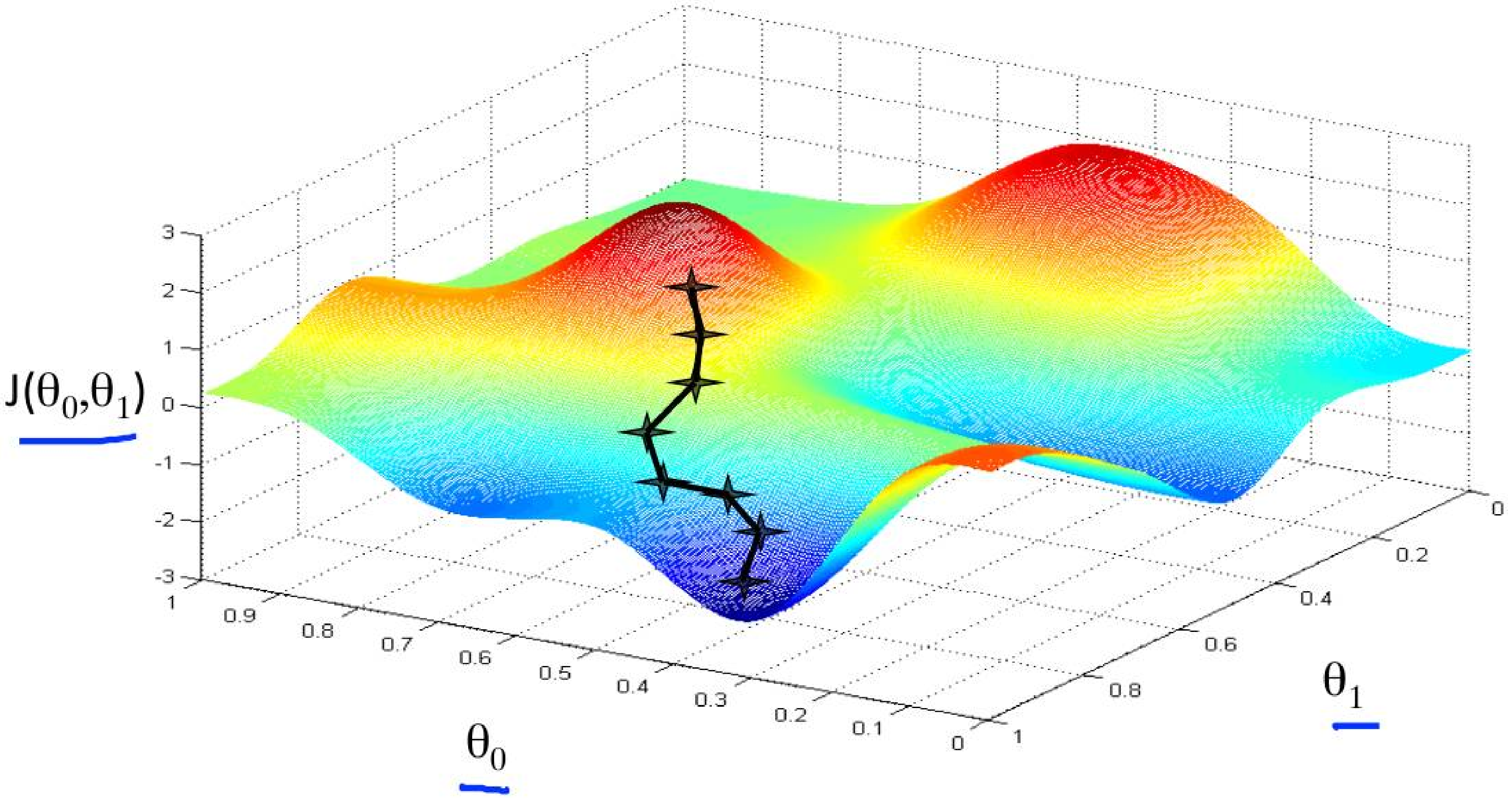
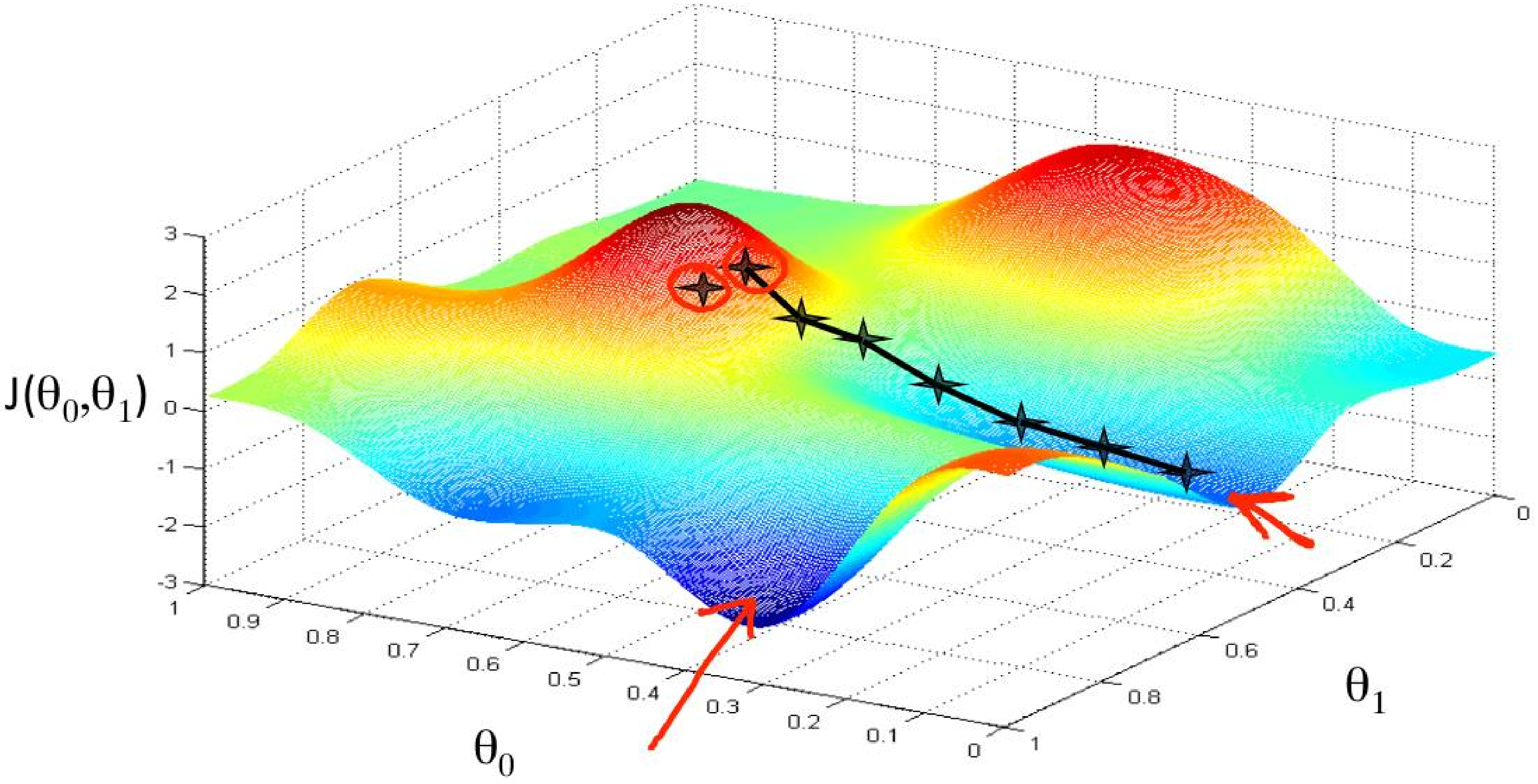


Case: When gradient descent reaches global minima



Case: When gradient descent does not reach global minima

Gradient descent algorithm

repeat until convergence {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad (\text{for } j = 0 \text{ and } j = 1)$$

}

Correct: Simultaneous update

$$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$
$$\theta_0 := \text{temp0}$$
$$\theta_1 := \text{temp1}$$

Gradient descent algorithm

Assignment | Truth assertion
$a := b$ | $a = b$
$a := a+1$ | ~~$a = a+1$~~

θ_0, θ_1

repeat until convergence {
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad (\text{for } j = 0 \text{ and } j = 1)$$
}

learning rate

Simultaneously update θ_0 and θ_1

Correct: Simultaneous update

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$
$\theta_0 := \text{temp0}$
$\theta_1 := \text{temp1}$

Incorrect:

$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$
$\theta_0 := \text{temp0}$
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$\theta_1 := \text{temp1}$

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Gradient descent algorithm

repeat until convergence {

$$\theta_j := \theta_j - \alpha \boxed{\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)} \quad \text{(simultaneously update } j = 0 \text{ and } j = 1)$$

}

learning rate

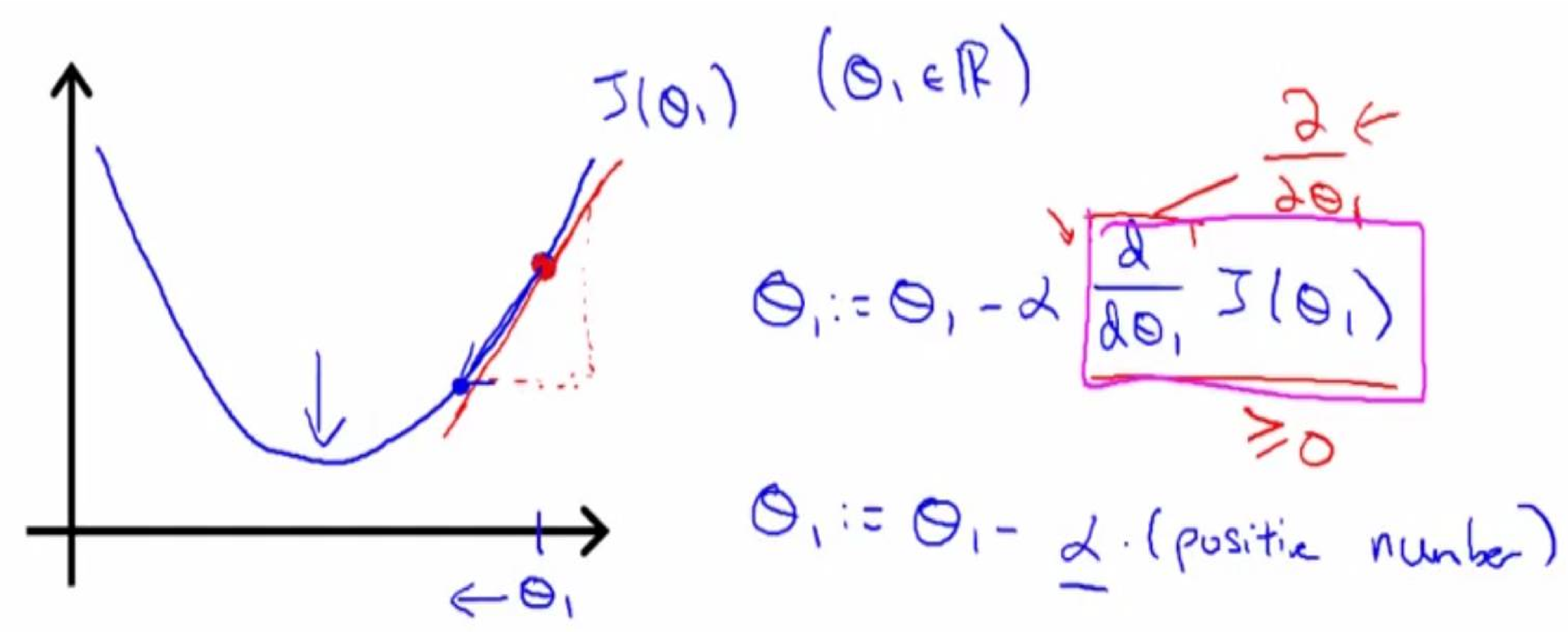
derivative

$\min_{\theta_1} J(\theta_1)$

$\theta_1 \in \mathbb{R}$.

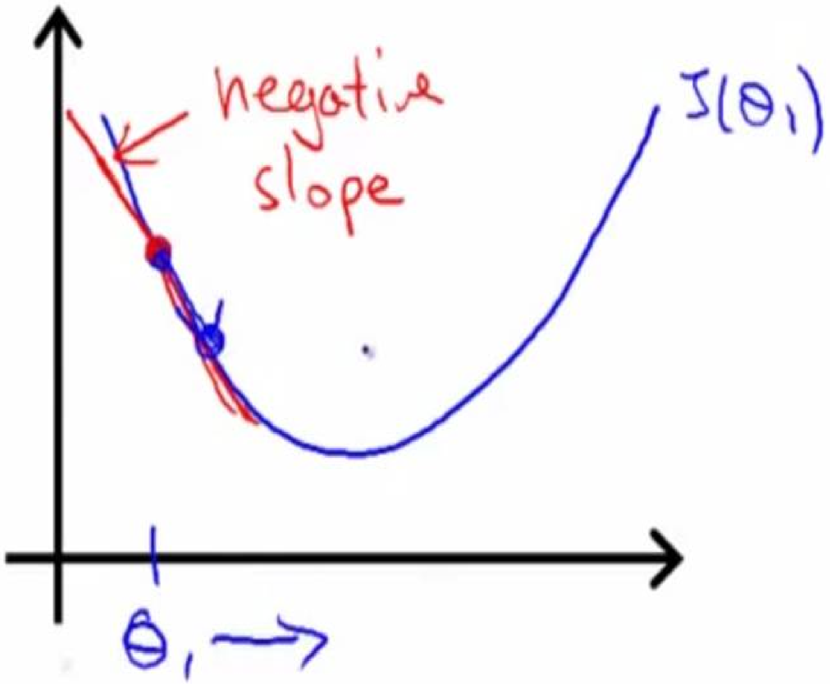
Assuming that J is a function of single parameter Θ_1

When slope is positive (move left).



Assuming that J is a function of single parameter Θ_1

When slope is negative (move right).



$$\frac{d}{d\theta_1} J(\theta_1) \le 0$$

$$\theta_1 := \theta_1 - \alpha \,(\text{negative number})$$

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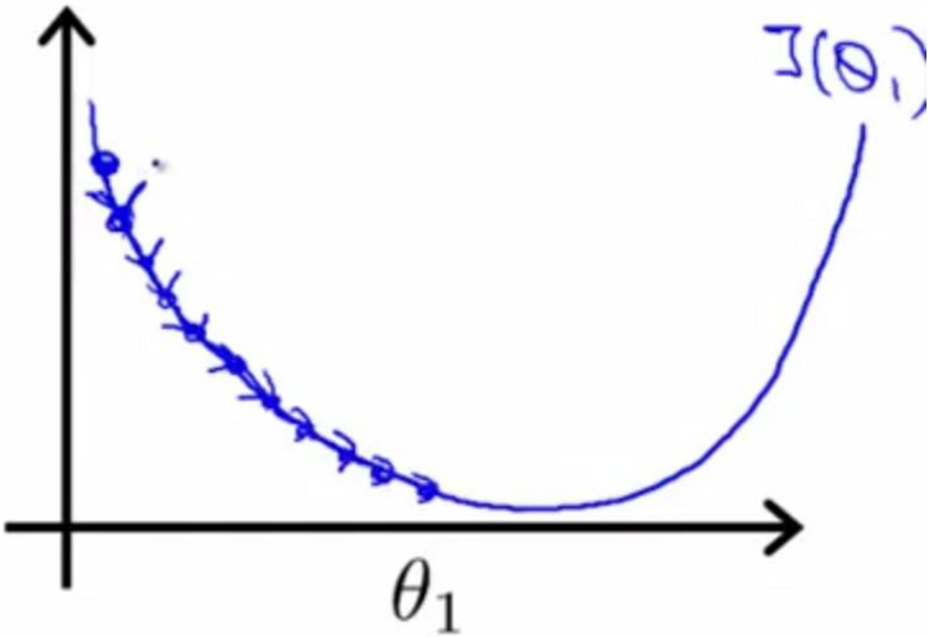
Effect of Learning Rate (α)

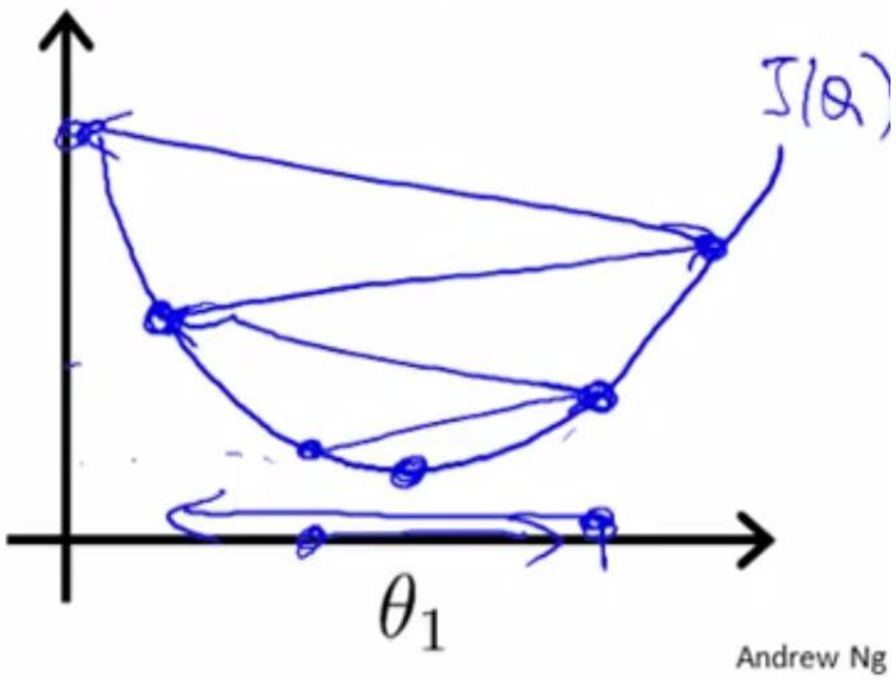
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If α is too small, gradient descent can be slow.

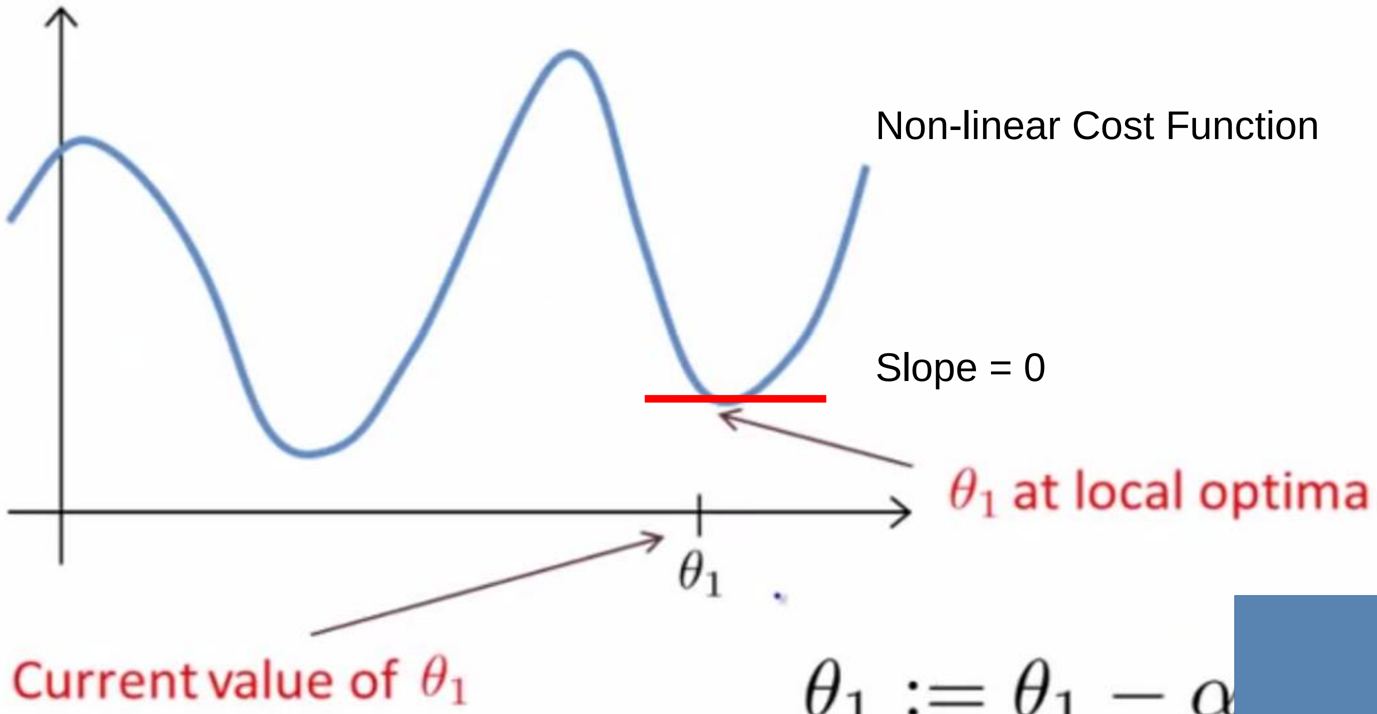


Effect of Learning Rate (α)

If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.



What will one step of gradient descent do if Θ_1 is already at the local minima?



Derivative = 0

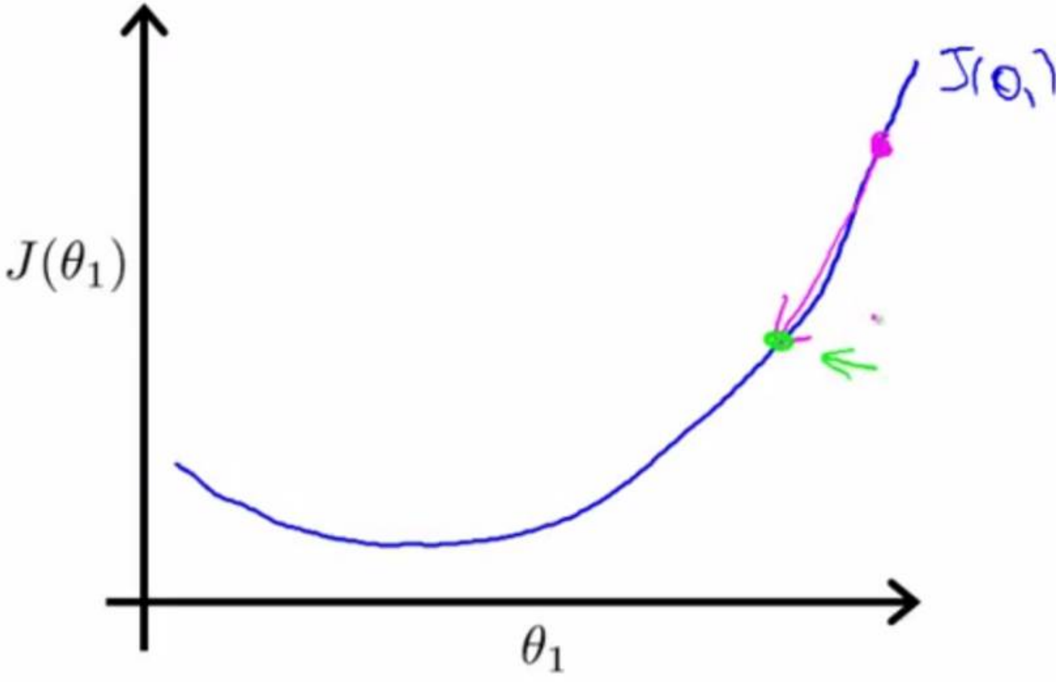
$$\theta_1 := \theta_1 - \alpha$$

Therefore, no change.

Gradient descent can converge to a local minimum, even with the learning rate α fixed.

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

As we approach a local minimum, gradient descent will automatically take smaller steps. So, no need to decrease α over time.



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Gradient descent can converge to a local minimum, even with the learning rate α fixed.

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

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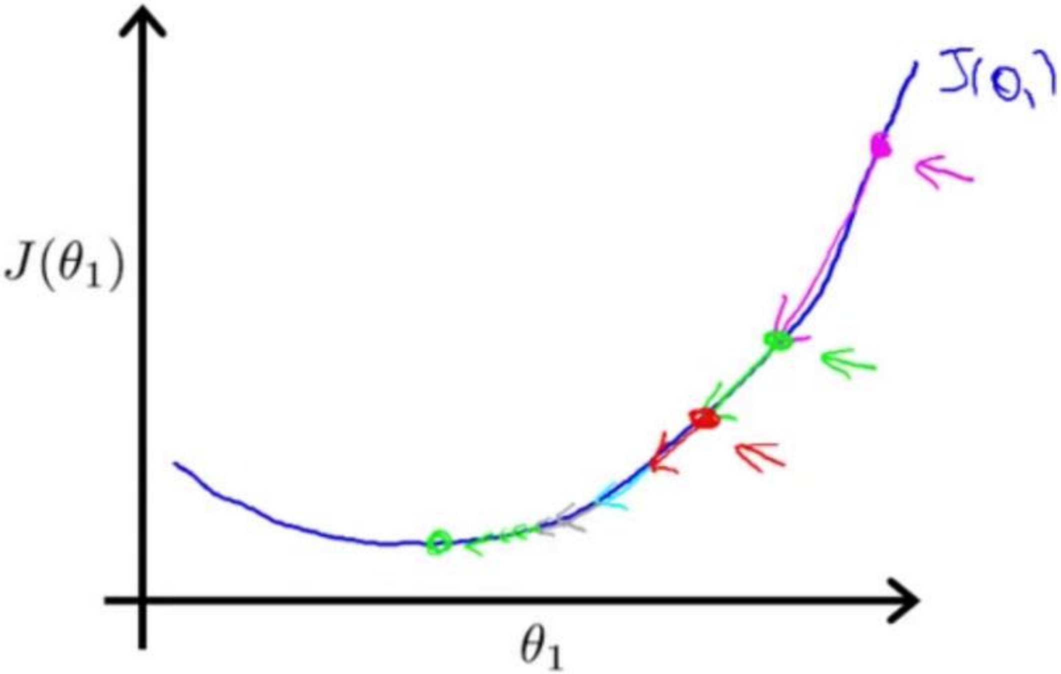

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Gradient Descent for linear regression

$$\frac{\partial}{\partial\theta_j} J(\theta_0, \theta_1) = \frac{\partial}{\partial\theta_j} \cdot \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

$$= \frac{\partial}{\partial\theta_j} \frac{1}{2m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)^2$$

$$\theta_0 \quad j = 0 : \frac{\partial}{\partial\theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)$$

$$\theta_1 \quad j = 1 : \frac{\partial}{\partial\theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)}$$

Gradient descent algorithm

repeat until convergence {

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}$$

}

Gradient descent algorithm

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

repeat until convergence {

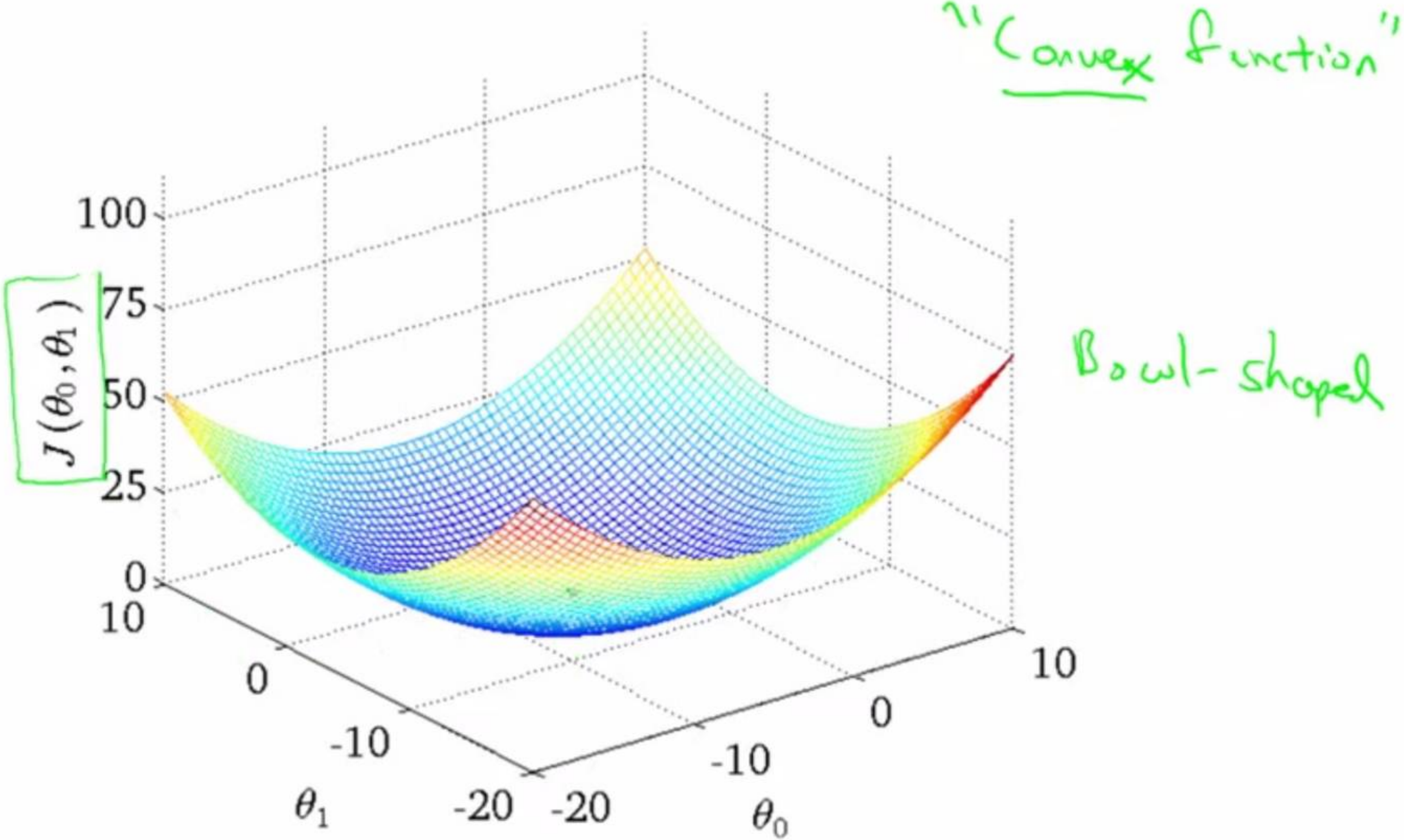
$$\theta_0 := \theta_0 - \alpha \boxed{\frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)}$$

$$\theta_1 := \theta_1 - \alpha \boxed{\frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}}$$

}

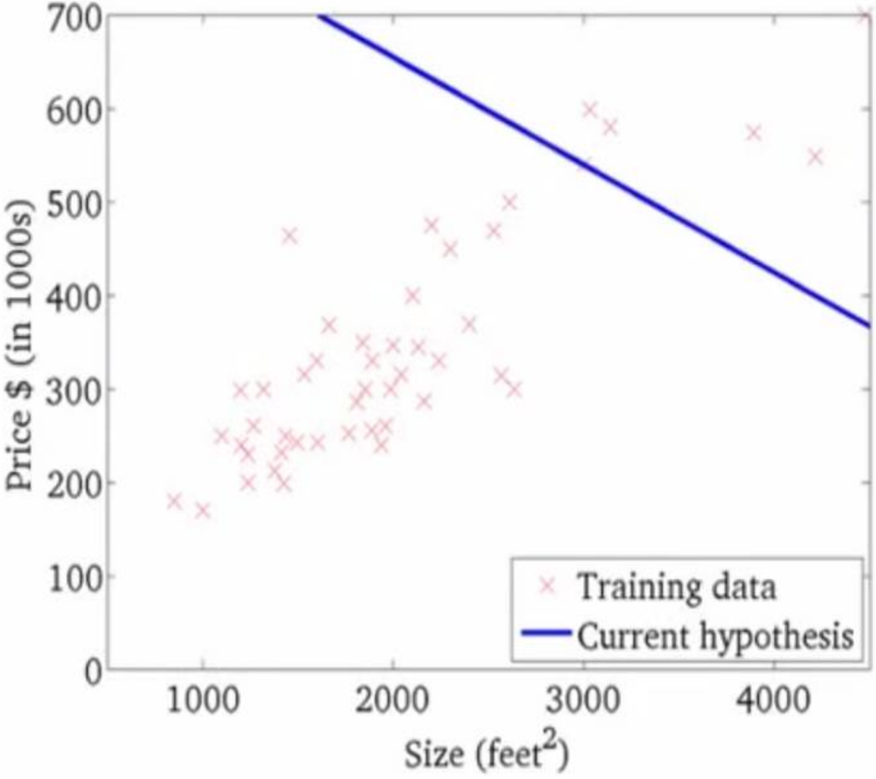
update θ_0 and θ_1 simultaneously

$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$


"Convex function"
Bowl-shaped
100
75
50
25
0
$J(\theta_0, \theta_1)$
10
0
-10
-20
θ_1
-20
-10
0
10
θ_0

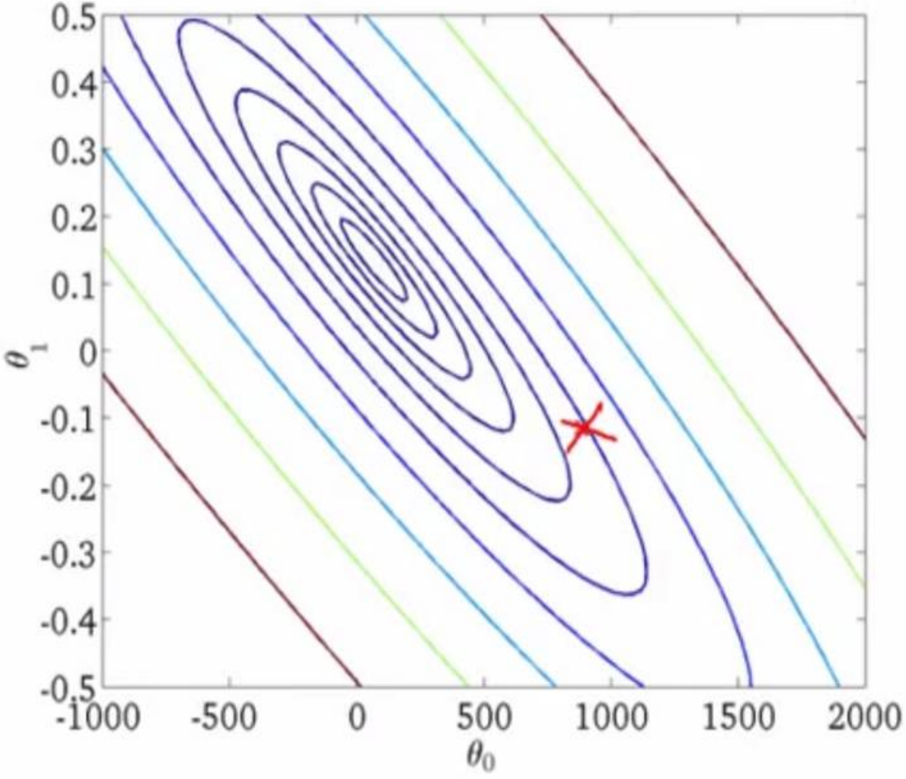
$h_\theta(x)$

(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)

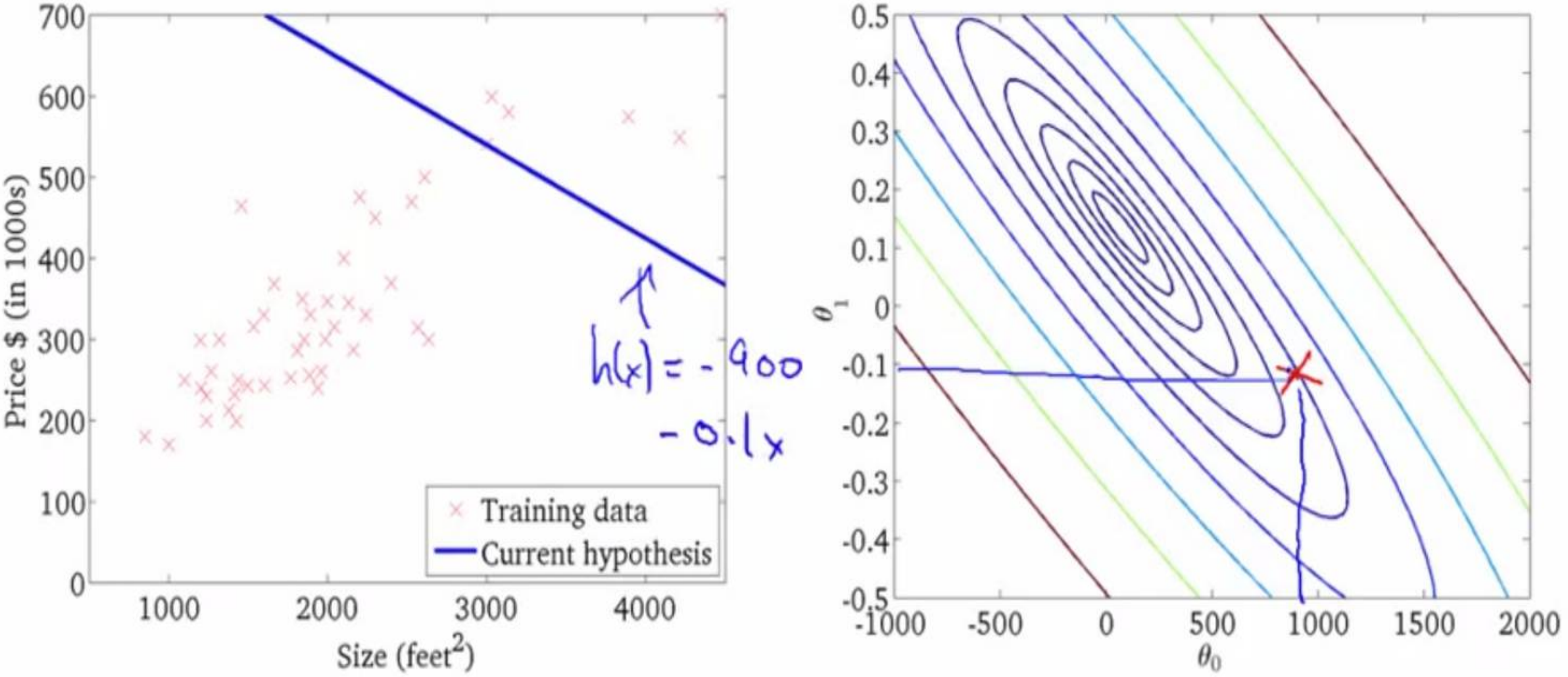


$h_\theta(x)$

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

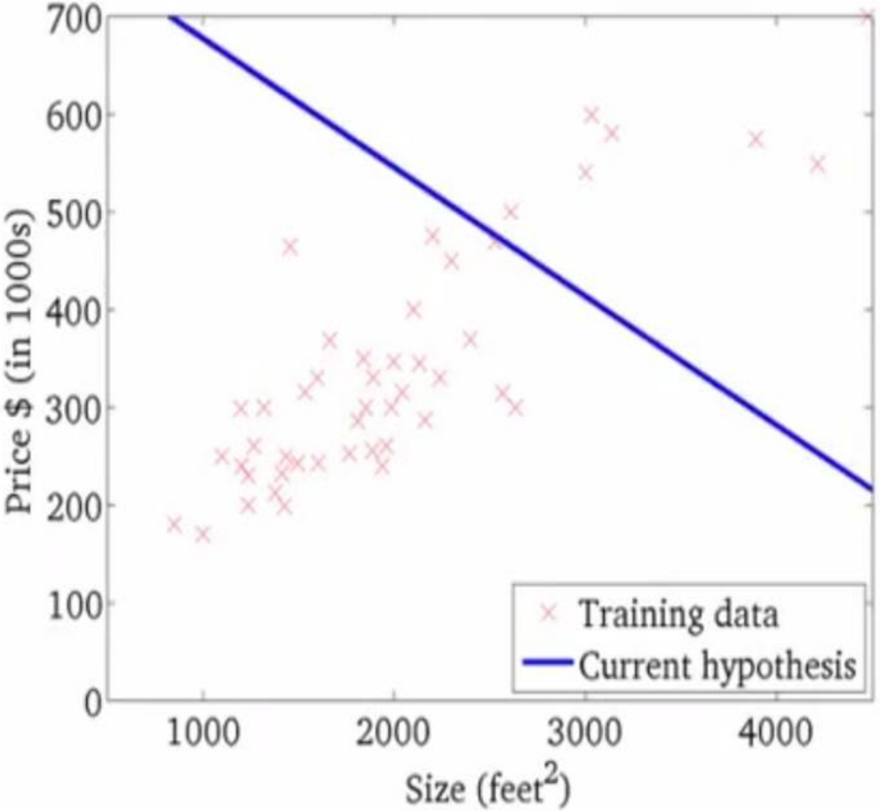
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



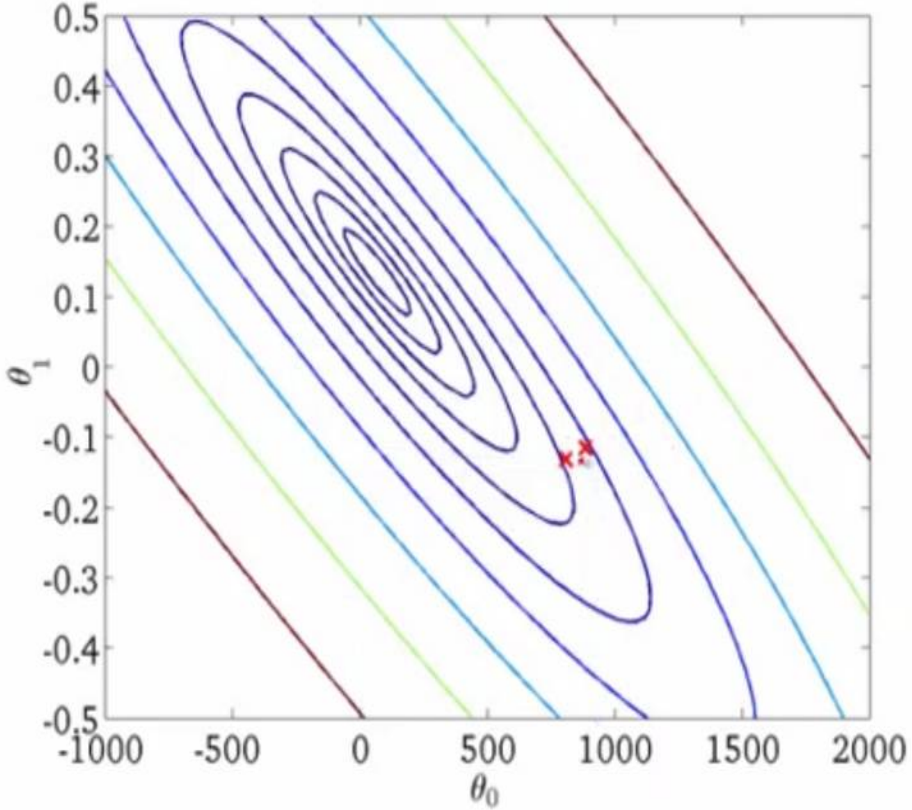
$$h_\theta(x)$$

(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)



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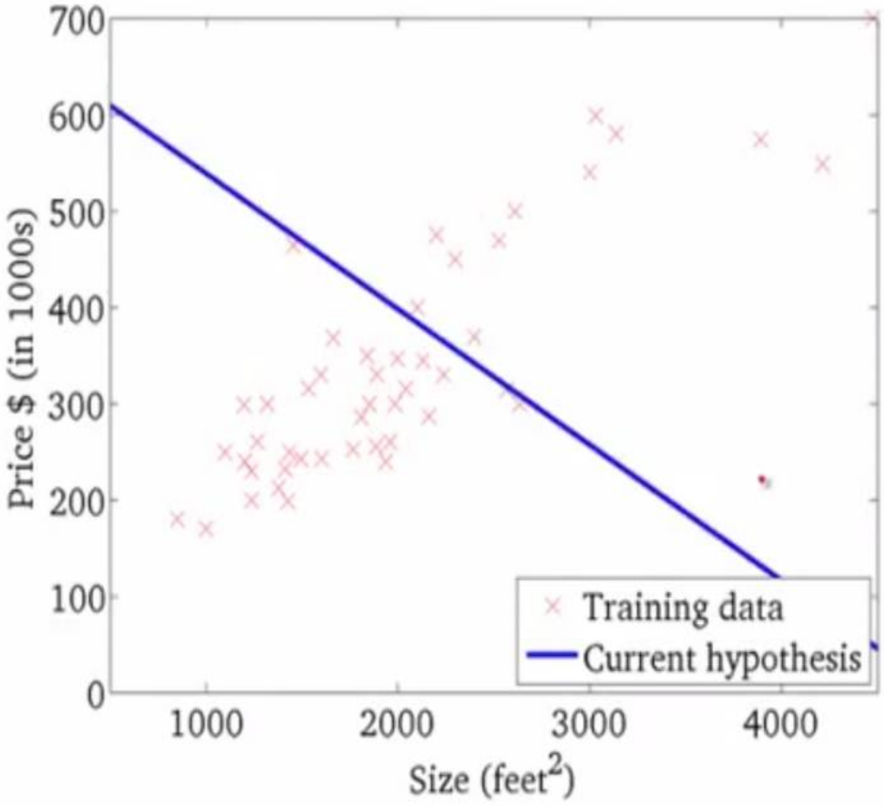
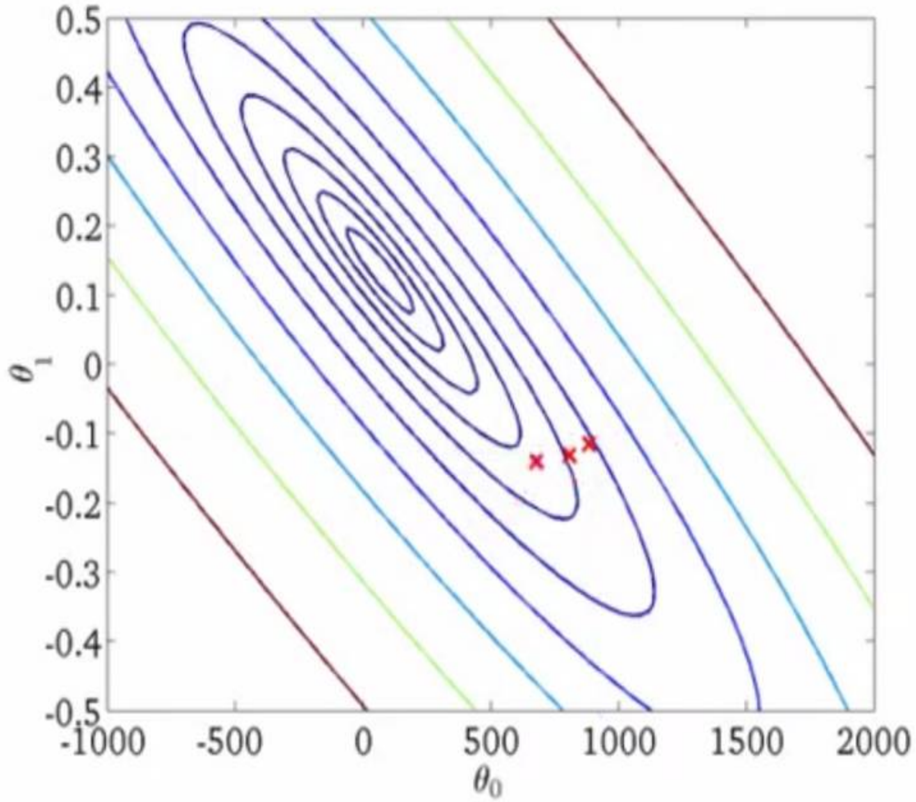


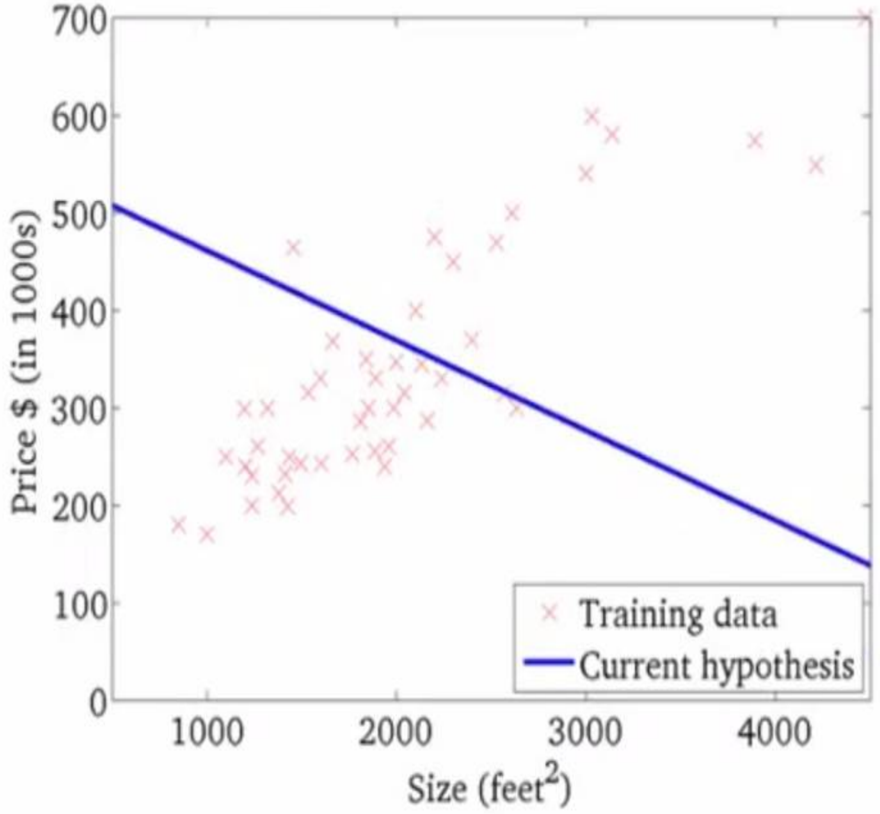
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



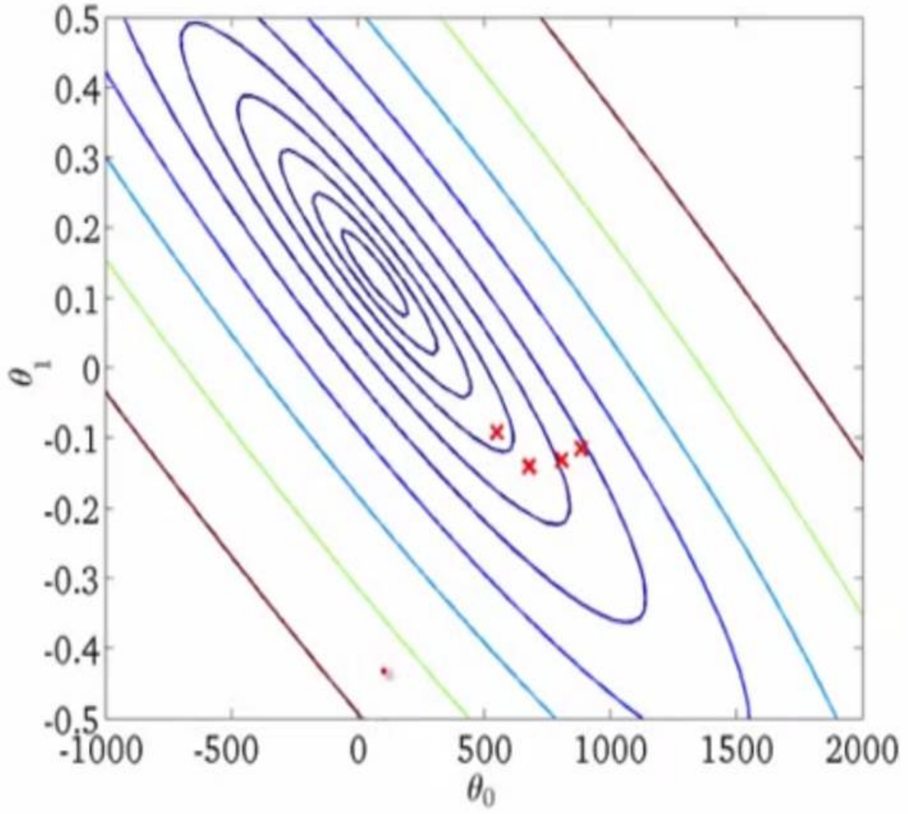
$h_\theta(x)$

(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)



$h_\theta(x)$

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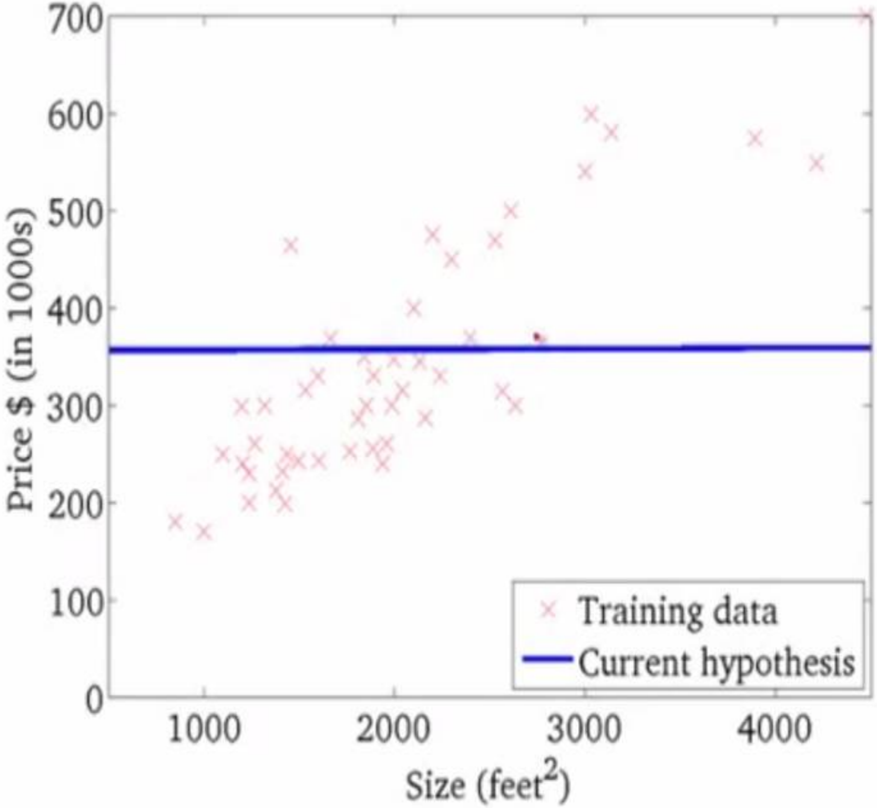
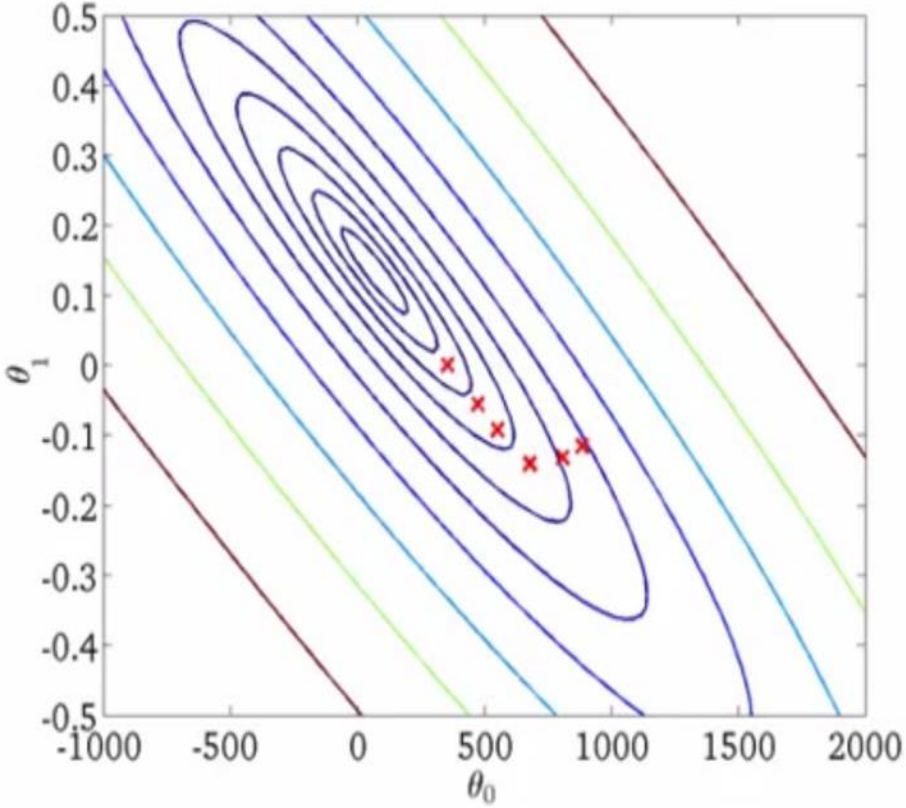


$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



$$h_\theta(x)$$

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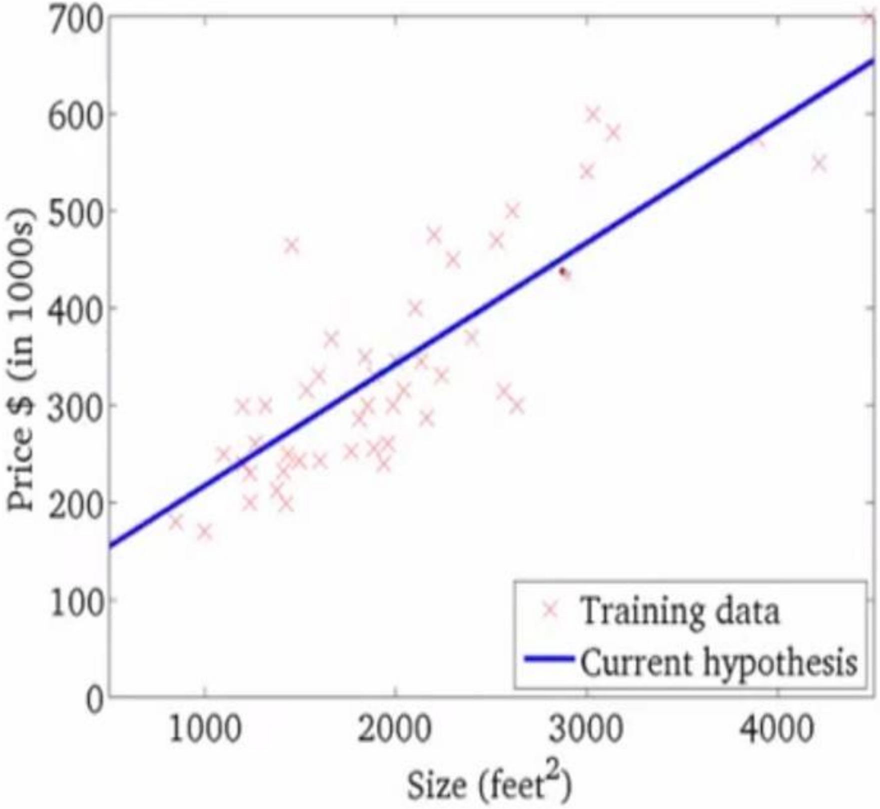
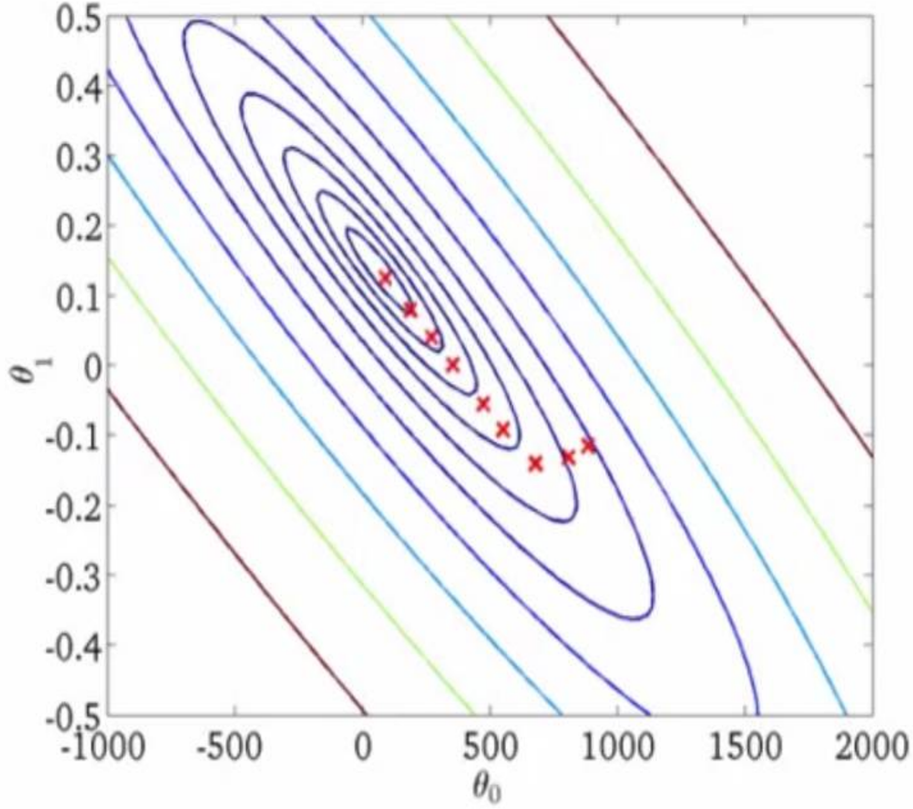


$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



Gradient Descent (Summary)

Aim: To Find (Θ_0, Θ_1) that minimizes height of the surface J(Θ).

- Start at some point.
- Find gradient and go down in the direction (steepest descent direction chosen)

- **Note**: For non-linear cost function with multiple minima points, it may get stuck at local minima
- For linear regression, there is no local optima. The cost function for linear regression is a Convex Function (bowl shaped). Convergence guaranteed.

"Batch" Gradient Descent

"Batch": Each step of gradient descent uses all the training examples.

$$\sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

If m is large (e.g., 1M examples), then computing the derivative becomes very slow, just to make a tiny update.

Stochastic Gradient Descent (SGD): Use only one random sample to compute the derivative and then update the parameters.

- It takes a noisy (random) path, but on average is headed towards the global minima.

- Used in practice for large datasets. Much **faster** in practice. May not quite converge to the exact global minima.

Multivariate LR: Using Multiple Features (Variables)

Multiple features (variables).

Size (feet^2) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

$m = 47$

Notation:

- n = number of features $n = 4$
- $x^{(i)}$ = input (features) of i^{th} training example.
- $x_j^{(i)}$ = value of feature j in i^{th} training example.

$$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix}$$

$$x_3^{(2)} = 2$$

Hypothesis (Multiple Features)

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$$

$$\text{E.g. } \underline{h_\theta(x)} = \underline{80} + \underline{0.1} x_1 + \underline{0.01} x_2 + 3x_3 - 2x_4$$

age

$$\rightarrow h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

For convenience of notation, define $\boxed{x_0 = 1.}$ $\quad (x_0^{(i)} = 1)$

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1} \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

$$\underbrace{\begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_n \end{bmatrix}}_{\theta^T} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

1 x (n + 1)

matrix

$\theta^T x$ $\qquad x$

$$h_\theta(x) = \theta_0 \overset{=1}{x_0} + \theta_1 x_1 + \cdots + \theta_n x_n$$

$$= \boxed{\theta^T x.}$$

Multivariate linear regression. $\leftarrow$

Gradient Descent for Multiple Variables

$x_0 = 1$

Hypothesis: $\underline{h_\theta(x) = \theta^T x = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n}$

Parameters: $\underline{\cancel{\theta_0, \theta_1, \ldots, \theta_n}}$ $\underline{\theta}$ n+1 - dimensional vector

Cost function:

$$\cancel{J(\theta_0, \theta_1, \ldots, \theta_n)} = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$J(\theta)$

Gradient descent:

Repeat $\{$

$$\rightarrow \theta_j := \theta_j - \alpha \boxed{\frac{\partial}{\partial \theta_j} \cancel{J(\theta_0, \ldots, \theta_n)} \; \underline{J(\theta)}}$$

$\}$ (simultaneously update for every $j = 0, \ldots, n$)

Gradient Descent

Previously (n=1):

Repeat $\{$

$$\theta_0 := \theta_0 - \alpha \underbrace{\boxed{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})}}_{\boxed{\frac{\partial}{\partial\theta_0}J(\theta)}}$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x^{(i)}$$

$x_1^{(i)}$

(simultaneously update θ_0, θ_1)

$\}$

New algorithm $(n \geq 2)$:

Repeat $\{$

$\frac{\partial}{\partial\theta_j} J(\theta)$

$$\theta_j := \theta_j - \alpha \boxed{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}}$$

(simultaneously update θ_j for $j = 0, \ldots, n$)

$\}$

Gradient Descent

Previously (n=1):

Repeat {

$$\theta_0 := \theta_0 - \alpha \underbrace{\boxed{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})}}_{\boxed{\frac{\partial}{\partial\theta_0}J(\theta)}}$$

$$\theta_1 := \theta_1 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x^{(i)}$$

$x_1^{(i)}$

(simultaneously update θ_0, θ_1)

}

New algorithm $(n \geq 2)$:

Repeat {

$\frac{\partial}{\partial\theta_j}J(\theta)$

$$\theta_j := \theta_j - \alpha\boxed{\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}}$$

(simultaneously update θ_j for $j = 0, \ldots, n$)

}

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_1 := \theta_1 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_1^{(i)}$$

$$\theta_2 := \theta_2 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_2^{(i)}$$

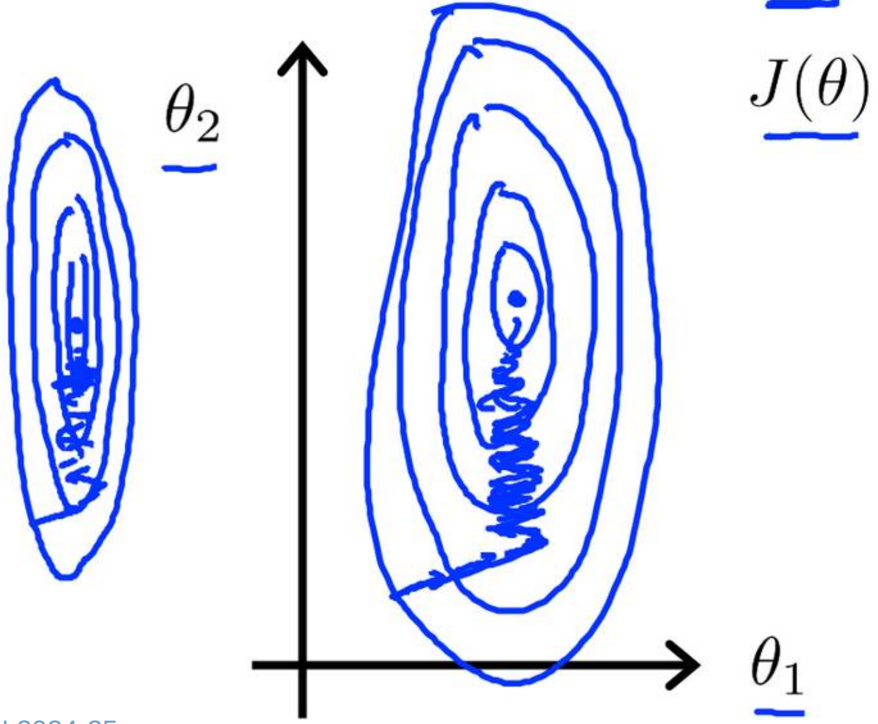
$\ldots$

Feature Scaling

Idea: Make sure features are on a similar scale.

E.g. x_1 = size (0-2000 feet^2)

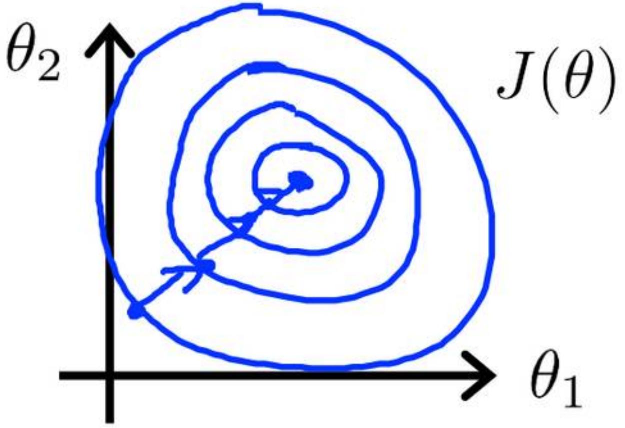
x_2 = number of bedrooms (1-5)



$$x_1 = \frac{\text{size (feet}^2)}{2000}$$

$$x_2 = \frac{\text{number of bedrooms}}{5}$$

$0 \le x_1 \le 1$ $\quad$ $0 \le x_2 \le 1$



Mean normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$).

E.g. $$x_1 = \frac{size - 1000}{2000}$$

$$x_2 = \frac{\#bedrooms - 2}{5}$$

$$-0.5 \le x_1 \le 0.5, -0.5 \le x_2 \le 0.5$$

$$x_1 \leftarrow \frac{x_1 - \mu_1}{s_1} \qquad \Big| \qquad x_2 \leftarrow \frac{x_2 - \mu_1}{s_2}$$

avg value of x_1 in training set

range (max - min)

(or standard deviation)

Gradient descent

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

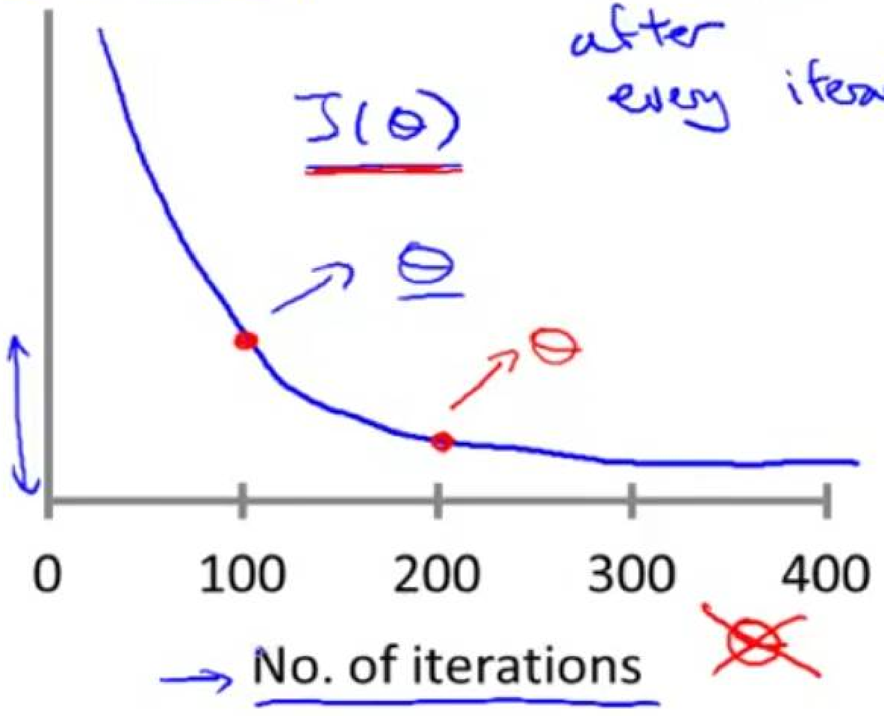
- "Debugging": How to make sure gradient descent is working correctly.

- How to choose learning rate α.

Making sure gradient descent is working correctly.

$\boxed{\min_\theta J(\theta)}$

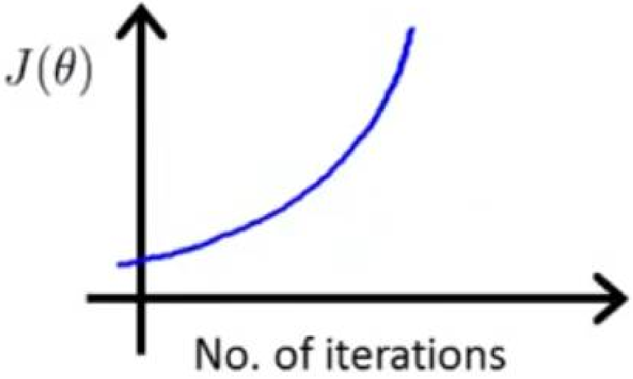
J(θ) should decrease after every iteration.



Example automatic convergence test:

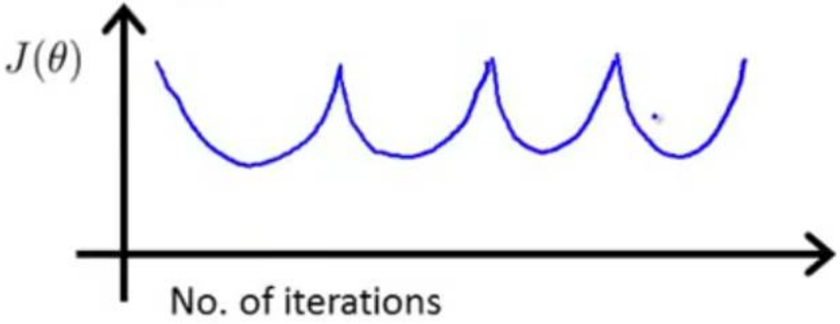
Declare convergence if $J(\theta)$ decreases by less than 10^{-3} in one iteration.

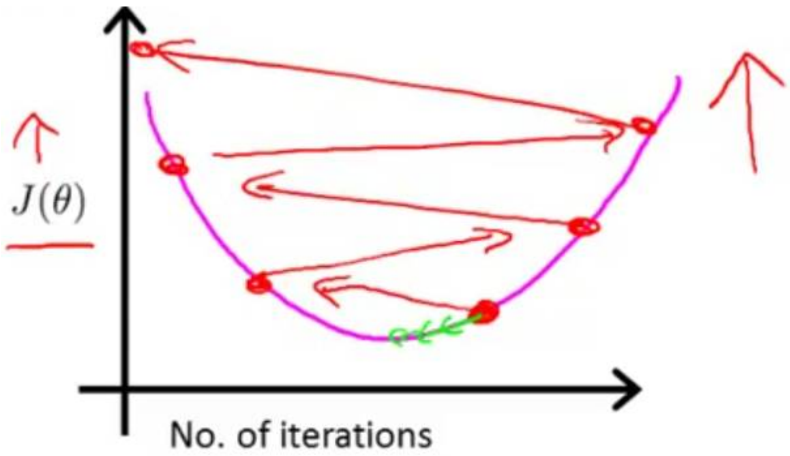
Making sure gradient descent is working correctly.



Gradient descent not working.

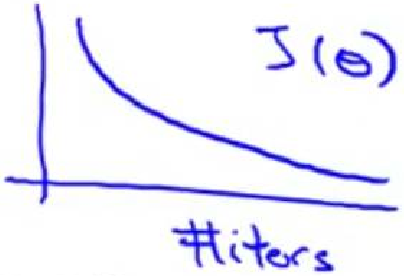
Use smaller α.





- For sufficiently small α, $J(\theta)$ should decrease on every iteration.
- But if α is too small, gradient descent can be slow to converge.

Summary:



- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge.

(Slow converge also possible)

To choose α, try

$$\ldots, 0.001, \quad , 0.01, \quad , 0.1, \quad , 1, \ldots$$

Features and Polynomial Regression

Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \underbrace{\boxed{frontage}}_{x_1} + \theta_2 \times \underbrace{\boxed{depth}}_{x_2}$$

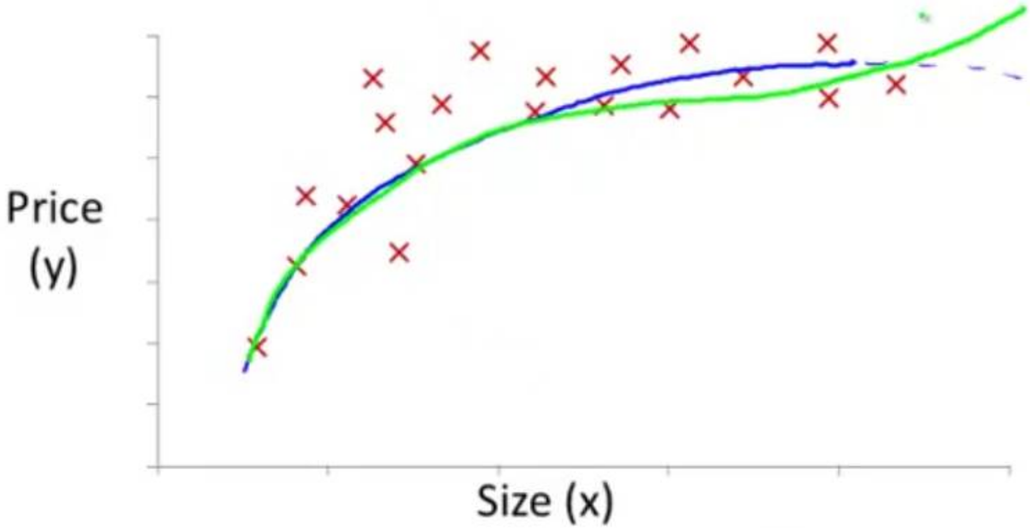
Area

$x = \underline{frontage * depth}$

$h_\theta(x) = \theta_0 + \theta_1 x$

↑ land area

Polynomial regression



$$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2$$

$$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
$$= \theta_0 + \theta_1(size) + \theta_2(size)^2 + \theta_3(size)^3$$

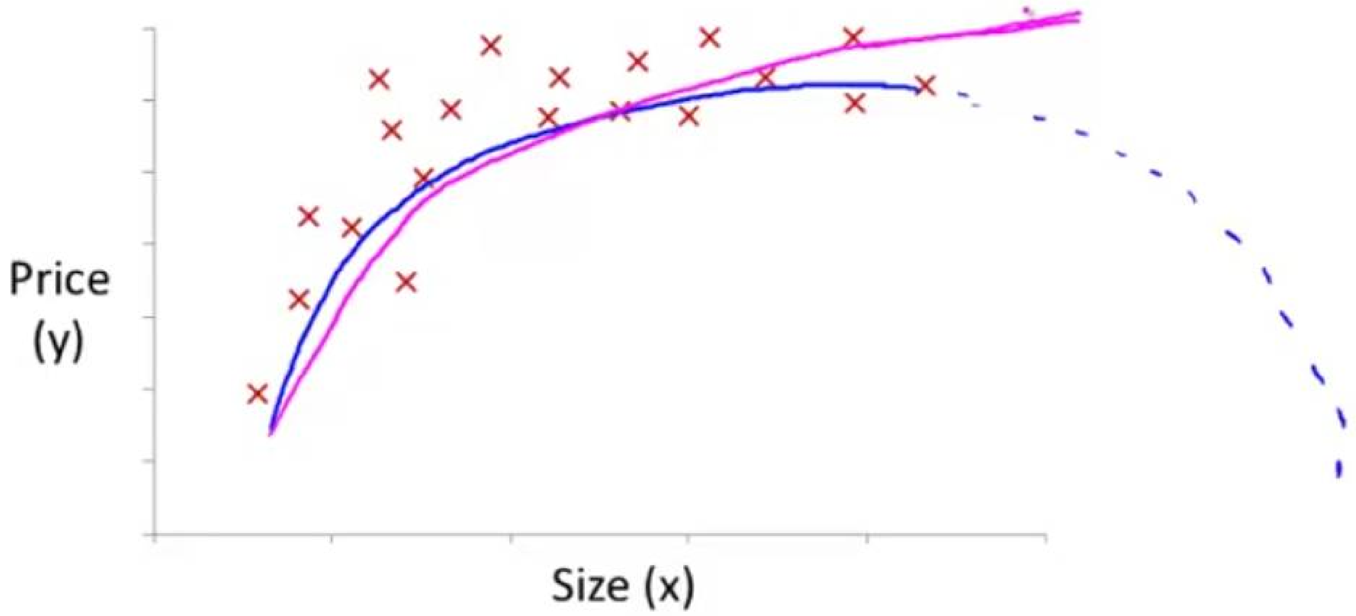
$$\rightarrow x_1 = (size)$$
$$\rightarrow x_2 = (size)^2$$
$$\rightarrow x_3 = (size)^3$$

Size: 1-1000

Size^2: 1-1000,000

Size^3: 1-10^9

Choice of features



$$h_\theta(x) = \theta_0 + \theta_1(size) + \theta_2(size)^2$$

$$h_\theta(x) = \theta_0 + \theta_1(size) + \theta_2\sqrt{(size)}$$

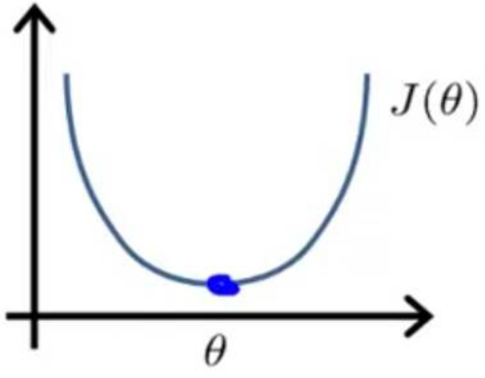
Normal Equation: Method to solve for Θ analytically

Intuition: If 1D ($\theta \in \mathbb{R}$)

$\rightarrow$ $J(\theta) = a\theta^2 + b\theta + c$

$$\frac{d}{d\theta} J(\theta) = \dots \overset{\text{set}}{=} 0$$

Solve for θ



$\theta \in \mathbb{R}^{n+1}$ $\qquad J(\theta_0, \theta_1, \dots, \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \cdots = 0 \quad \text{(for every } j\text{)}$$

Solve for $\theta_0, \theta_1, \dots, \theta_n$

Examples: $m = 4.$

x_0	Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix} \qquad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

m x (n+1)

m-dimensional vector

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

m **examples** $(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$ **;** n **features.**

$$x^{(i)} = \boxed{\begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}} \in \mathbb{R}^{n+1}$$

$$X = \begin{bmatrix} \text{---} (x^{(1)})^T \text{---} \\ \text{---} (x^{(2)})^T \text{---} \\ \vdots \\ \text{---} (x^{(m)})^T \text{---} \end{bmatrix}$$

(design matrix)

$m \times (n+1)$

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

Question

- Which of the following is/are True w.r.t. normal equation?
  - It may not have a solution.
  - It may have a unique solution.
  - It may have infinite solutions.
  - It is the least squares solution of $Ax = b$

Homework

- Derivation of Normal Equation.
- In which cases will a unique solution be not available using the Normal Equation (for linear regression).
- Is feature scaling necessary when using a Normal Equation to solve the linear regression task. (Hint: Are iterations needed.)

m training examples, n features.

Gradient Descent	Normal Equation
• Need to choose α.	• No need to choose α.
• Needs many iterations.	• Don't need to iterate.
• Works well even when n is large.	• Need to compute $\boxed{(\boxed{X^TX})^{-1}}$ $n \times n$ $O(n^3)$
$n = 10^6$	• Slow if n is very large.
	$n = 100$
	$n = 1000$
	$n = 10000$

References

- Gradient Descent Playground

  https://uclaacm.github.io/gradient-descent-visualiser/

- Stanford CS229 Machine Learning Course by Andrew Ng.

End of Lecture