Machine Learning and Pattern Recognition

A High Level Overview

Prof. Anderson Rocha

(Main bulk of slides kindly provided by **Prof. Sandra Avila**
and largely based on other materials as well (e.g., Andrew Ng's))

Institute of Computing (IC/Unicamp)

MC886/MO444

House Price Prediction

$ 70 000

https://www.youtube.com/watch?v=IpGxLWOIZy4

House Price Prediction

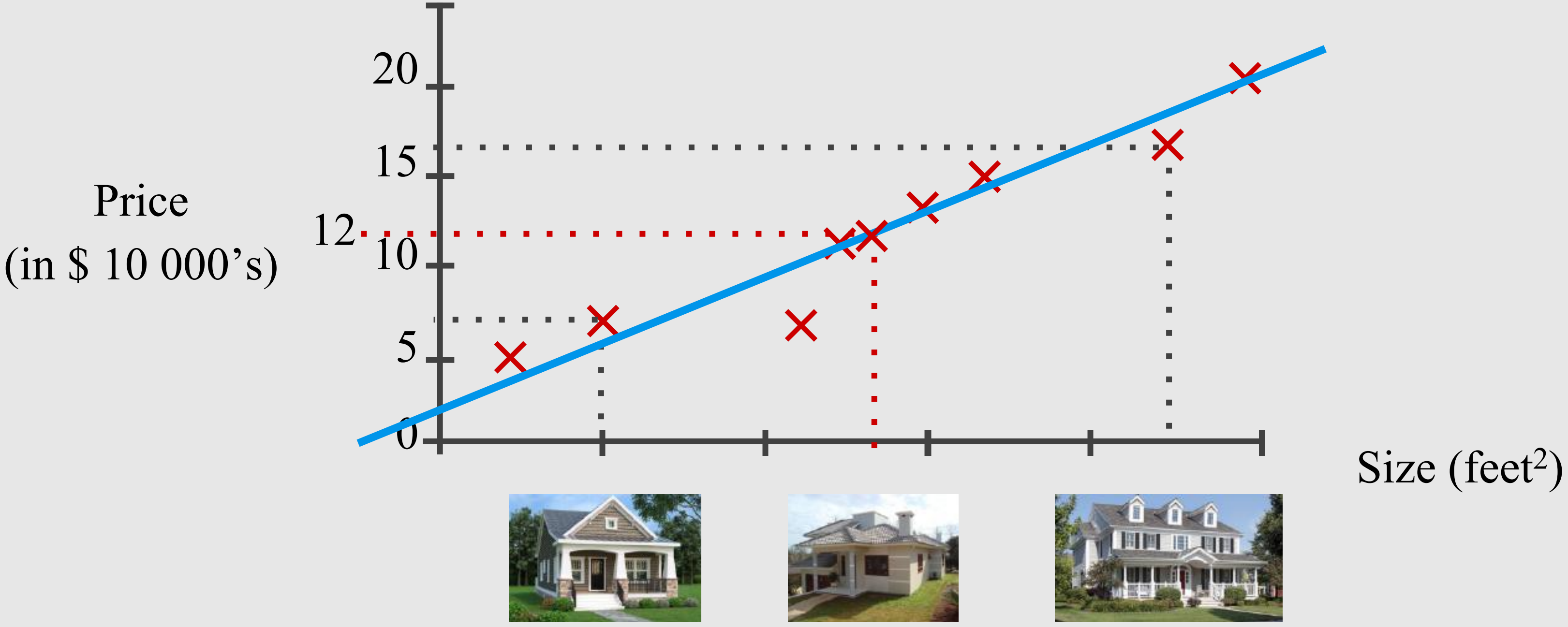
$ 160 000

House Price Prediction

???

House Price Prediction

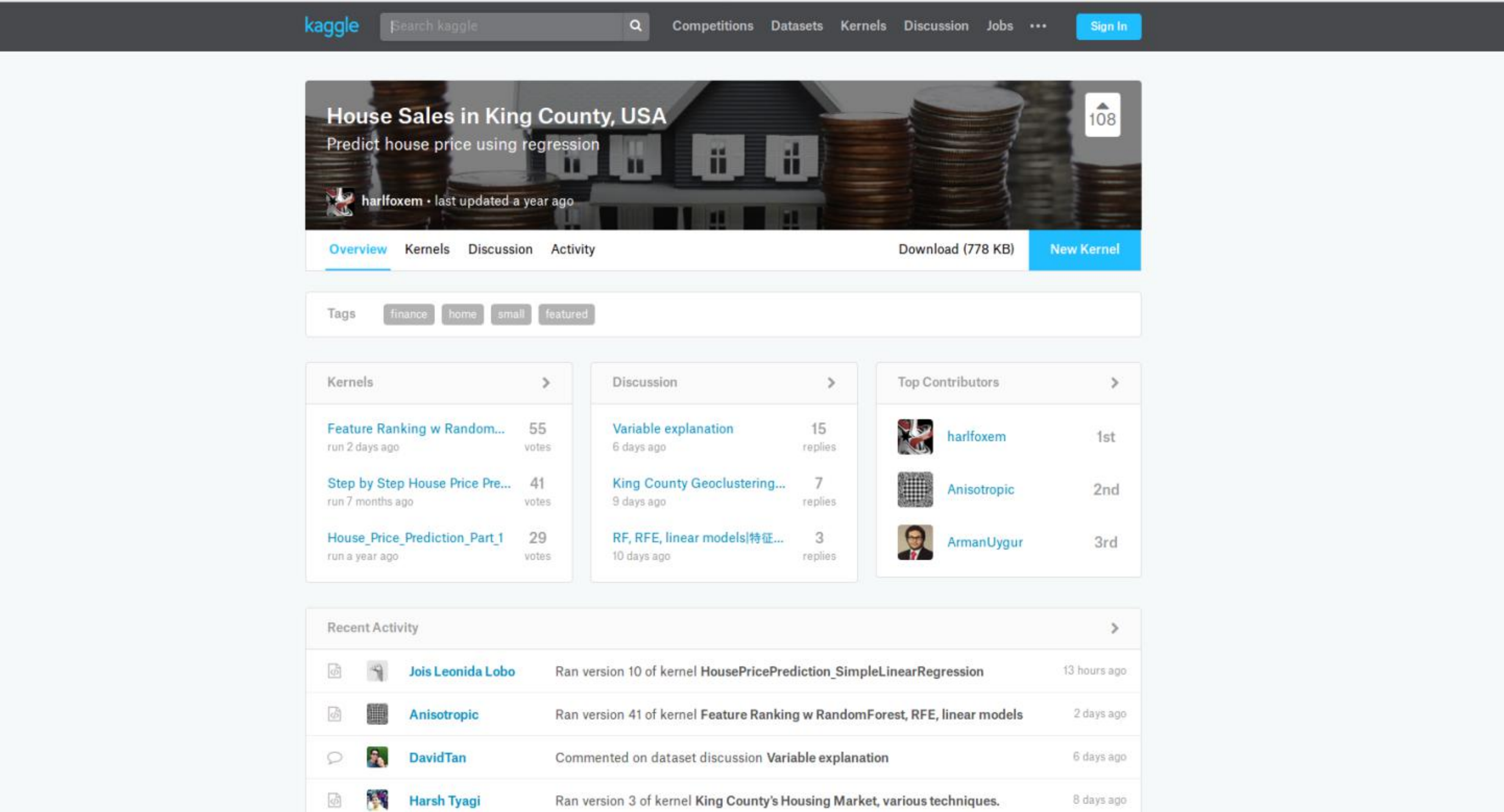
Linear Regression



Today’s Agenda

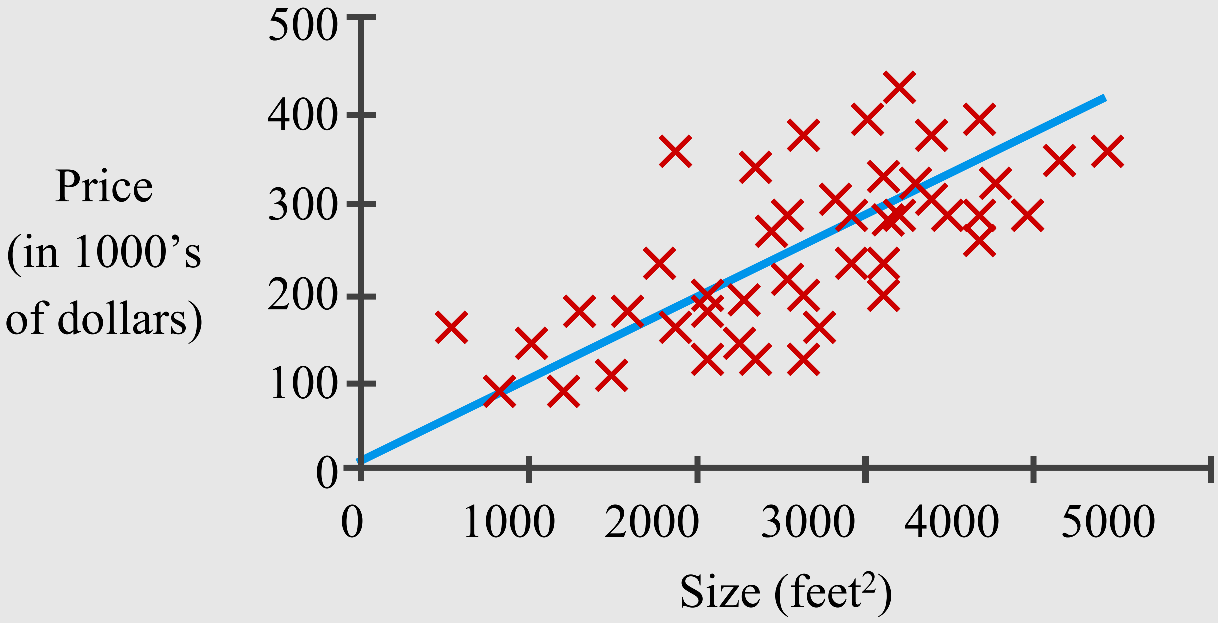
- Linear Regression with One Variable
  - Model Representation
  - Cost Function
  - Gradient Descent
- Linear Regression with Multiple Variables
  - Gradient Descent for Multiple Variables
  - Feature Scaling
  - Learning Rate
  - Features and Polynomial Regression
  - Normal Equation

Model Representation



https://www.kaggle.com/harlfoxem/housesalesprediction

Housing Prices



Supervised Learning

Given the "right answer" for each example in the data.

Regression Problem

Predict real-valued output

Training set of housing prices

Size in feet^2 (x)	**Price (\$) in 1000's (y)**
2104	460
1416	232
1534	315
852	178
…	…

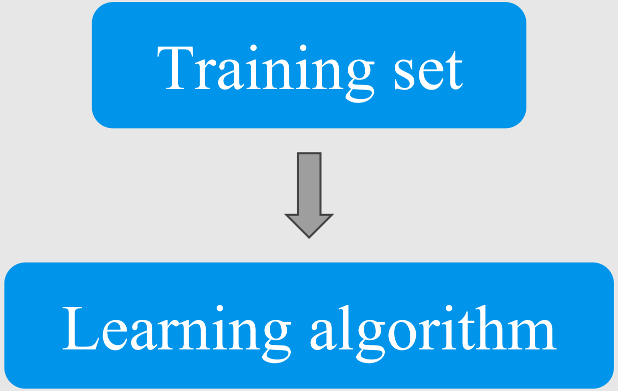
Notation:

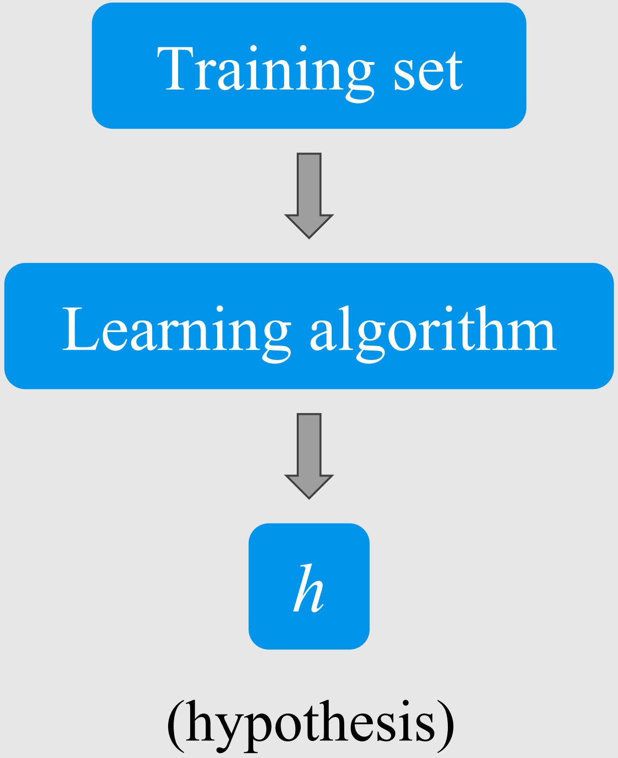
m = Number of training examples

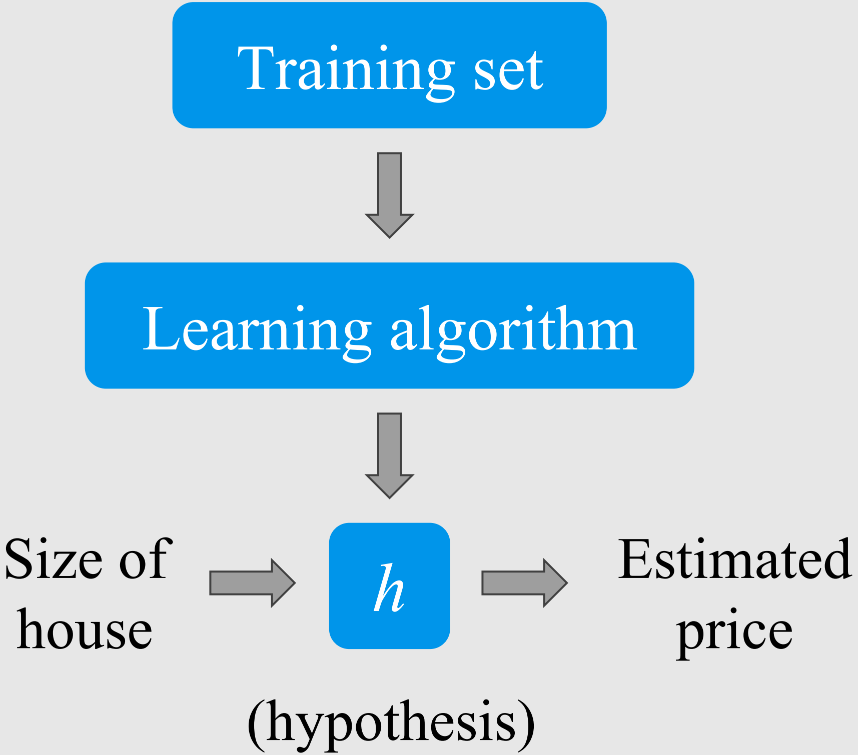
x's = "input" variable / features

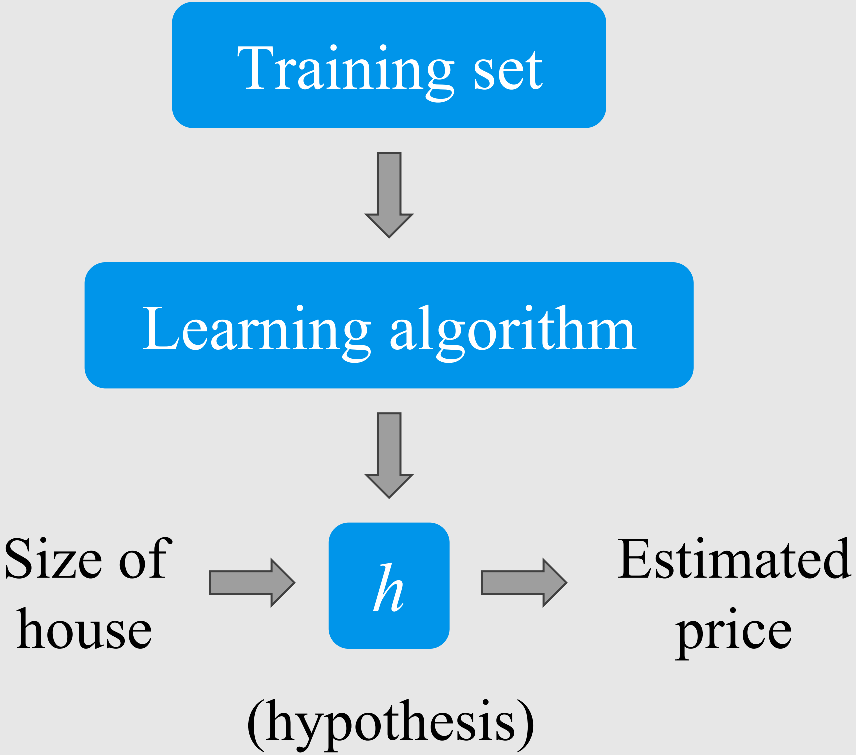
y's = "output" variable / "target" variable

Training set


Training set
Learning algorithm

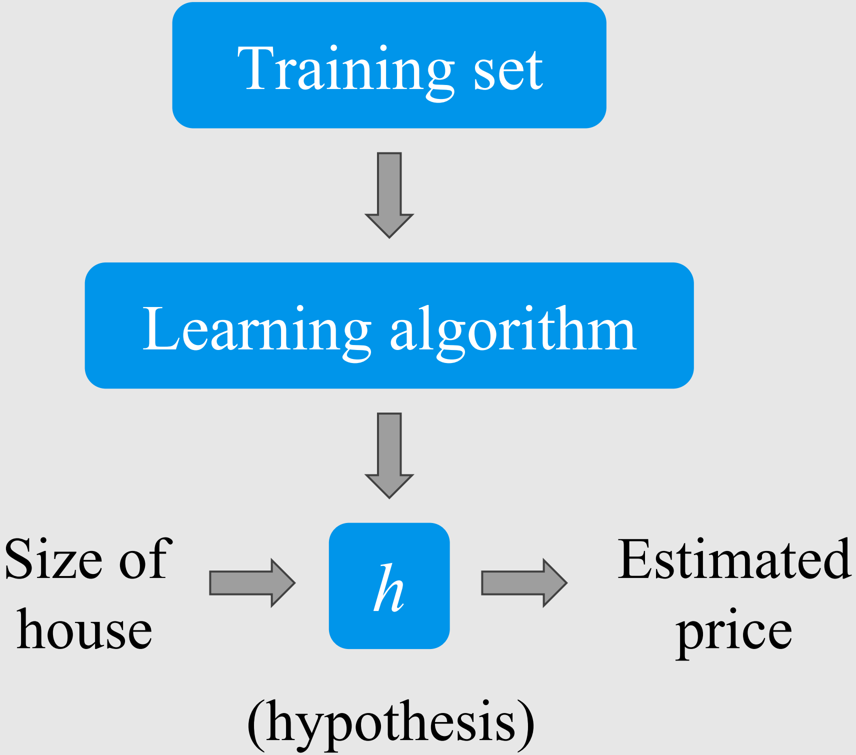

Training set
Learning algorithm
h
(hypothesis)


Training set
Learning algorithm
Size of house
h
Estimated price
(hypothesis)



***h* maps *x*’s to *y*’s**

How do we represent h ?



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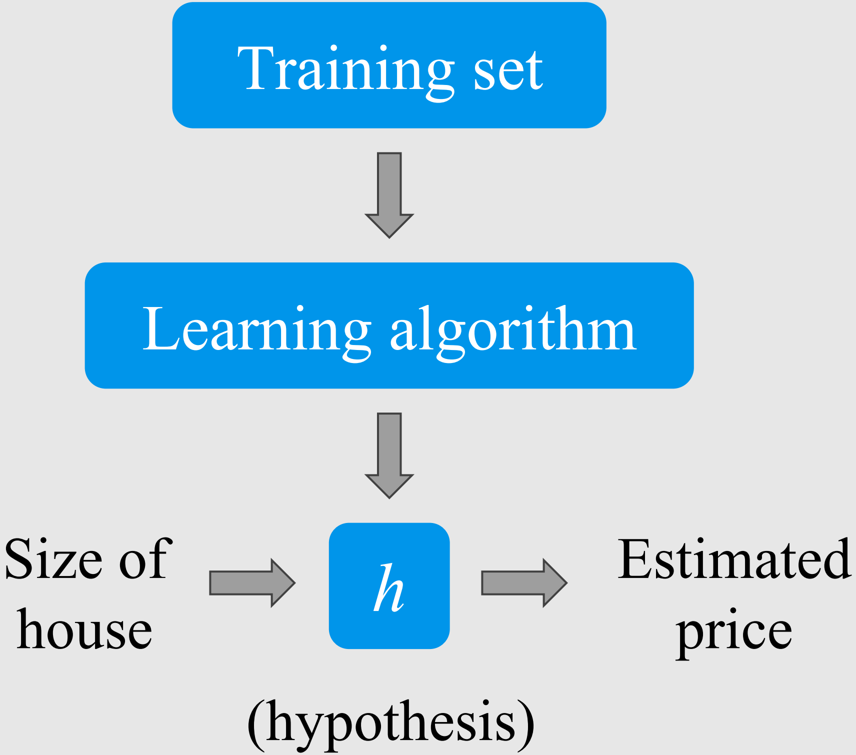
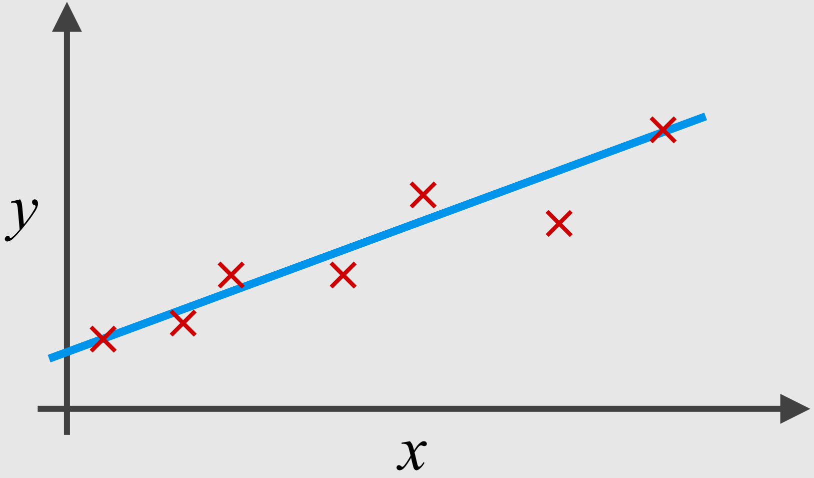
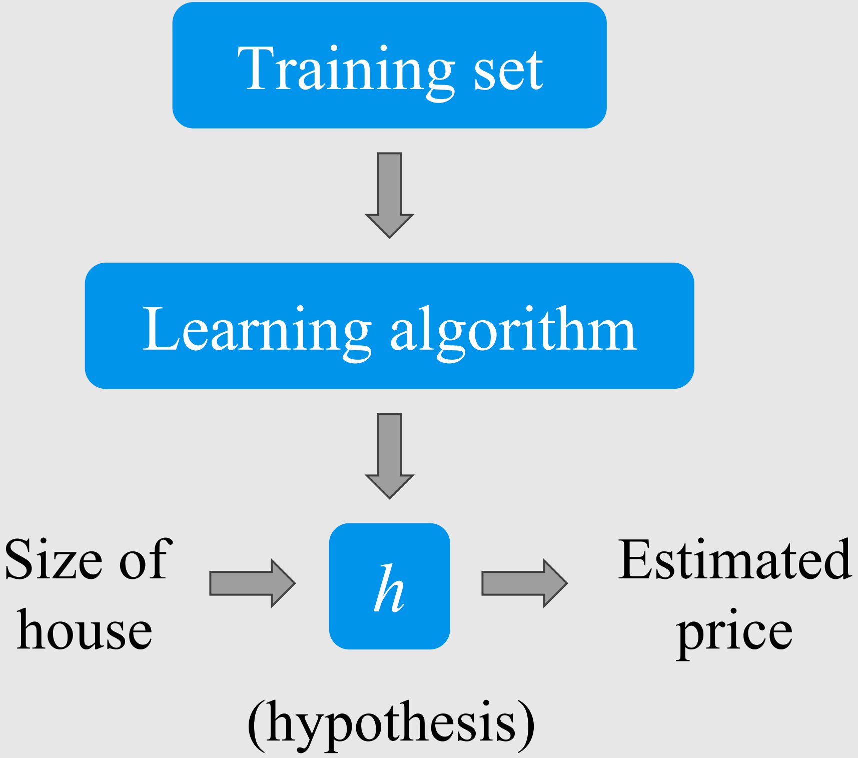


***h* maps *x*'s to *y*'s**

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



How do we represent *h* ?



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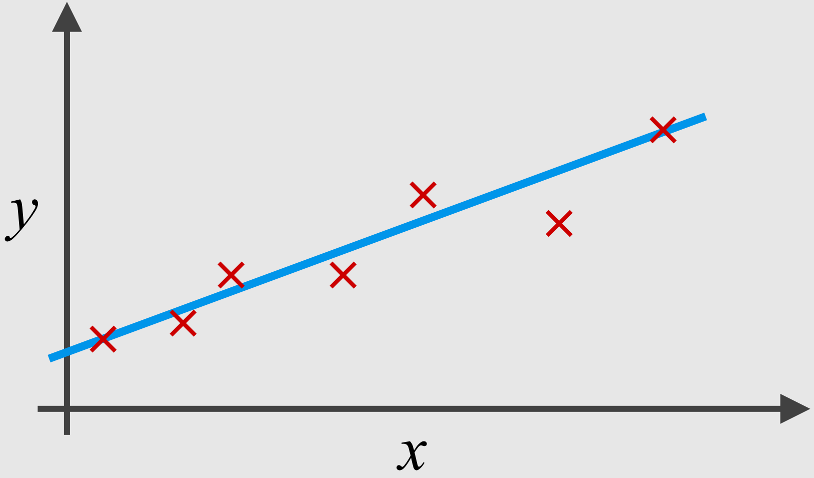


Linear regression with one variable.
Univariate linear regression.

Cost Function

Training Set

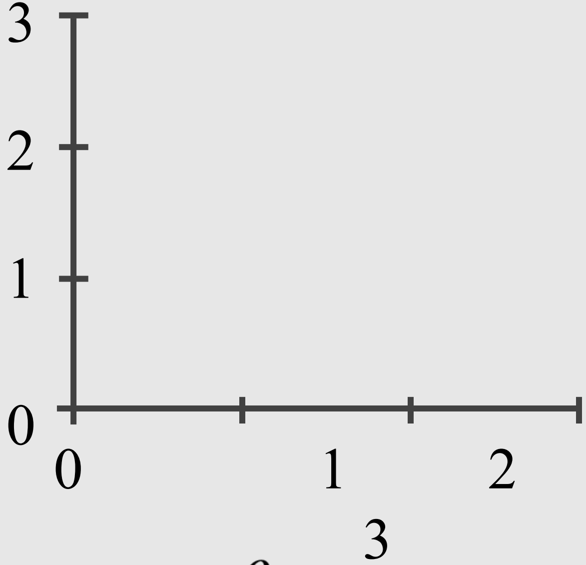
Size in feet² (x)	**Price ($) in 1000's ($y$)**
2104	460
1416	232
1534	315
852	178
...	...

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

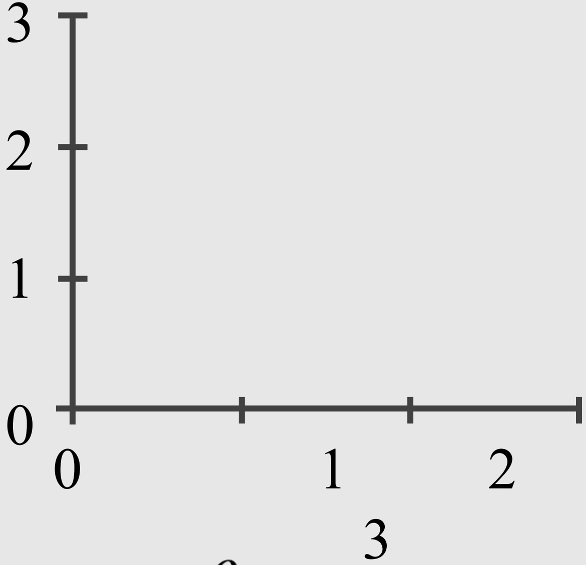
θ_i's: Parameters

How to choose θ_i's ?

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



$\theta_0 = 1.5$
$\theta_1 = 0$



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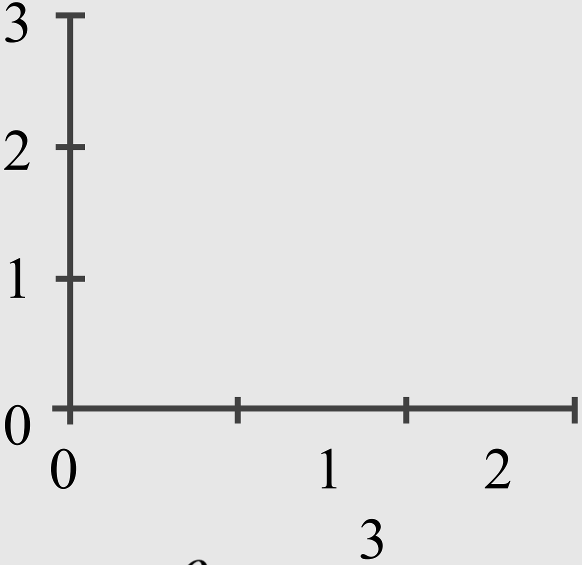

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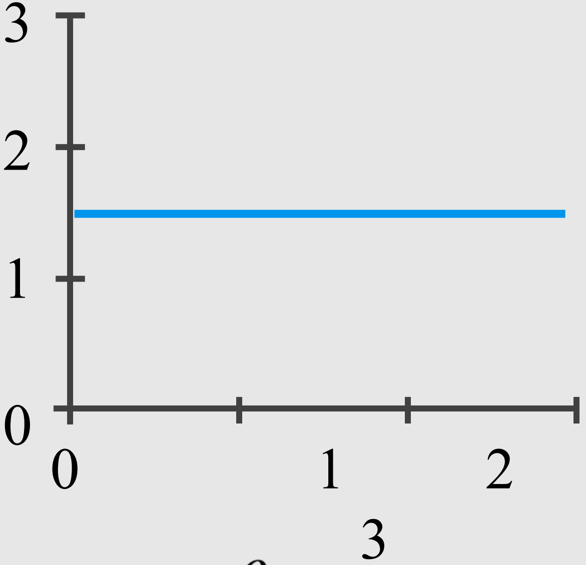
$$h_\theta(x) = \theta_0 + \theta_1 x$$



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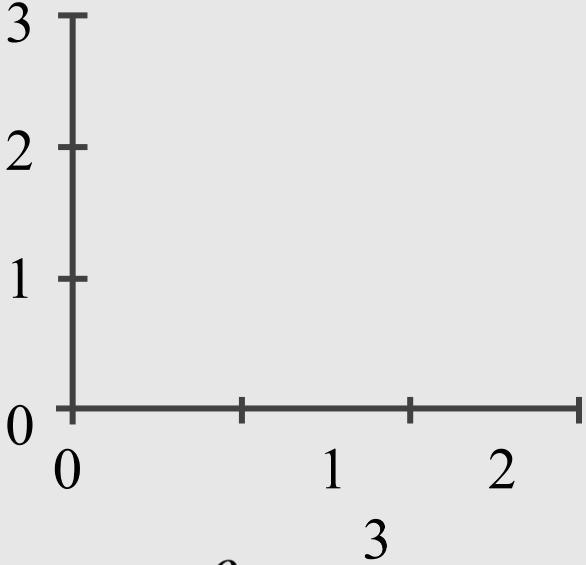

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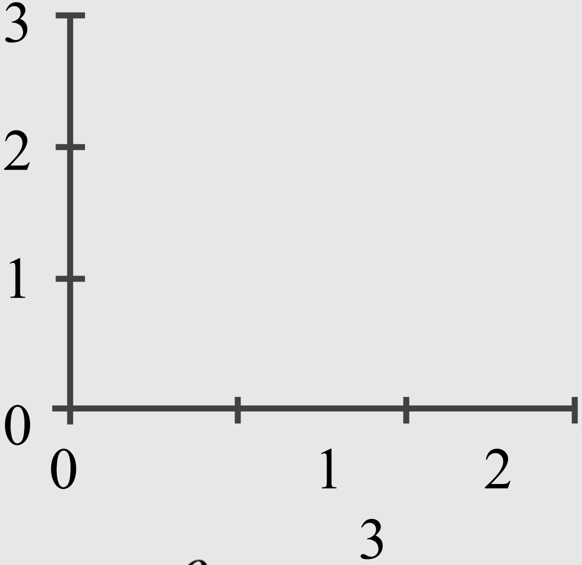

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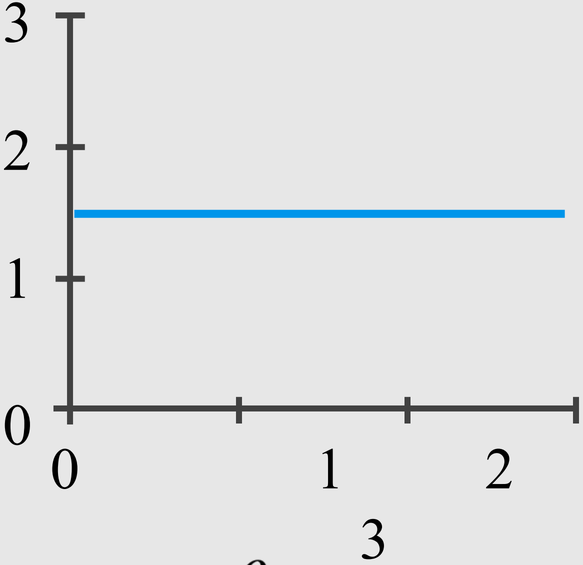

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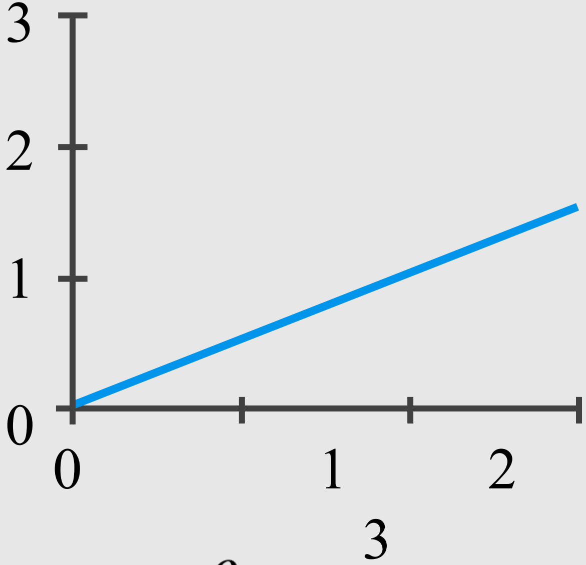

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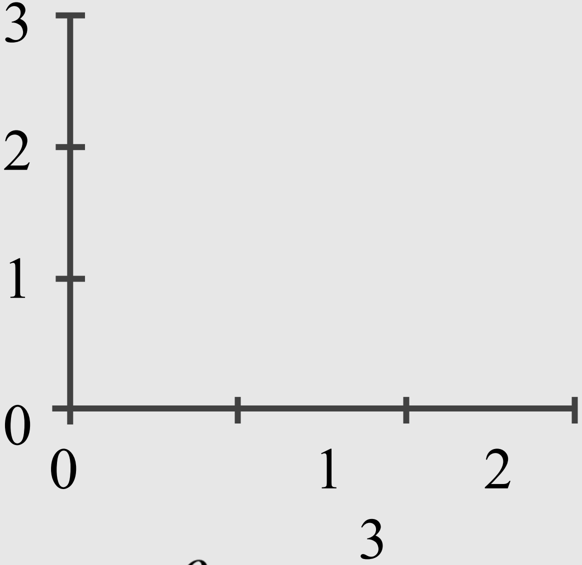

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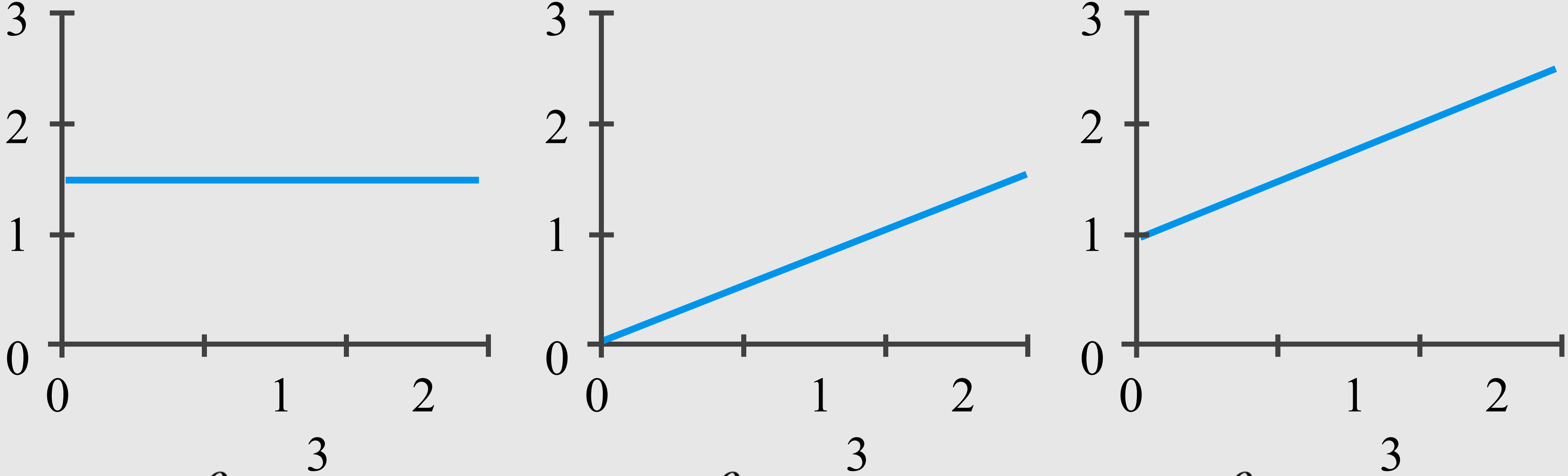
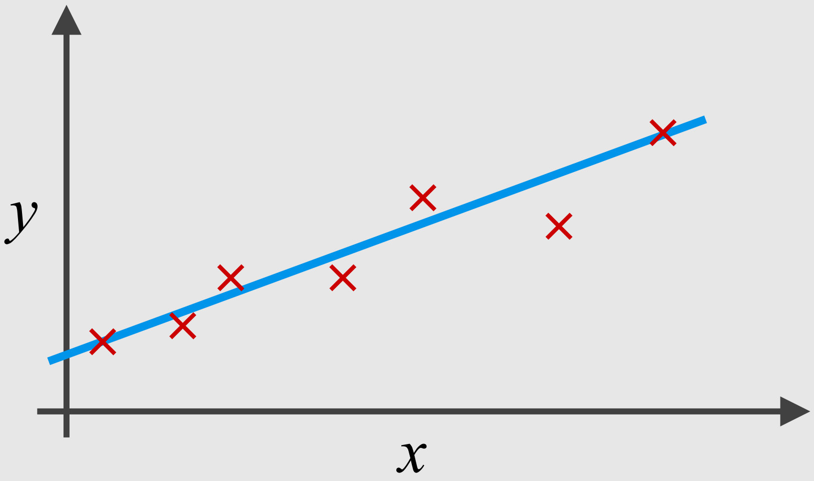


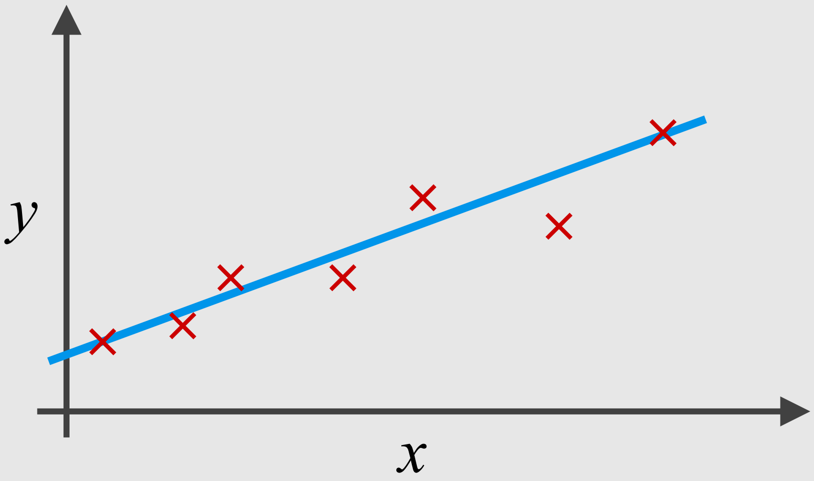
$\theta_0 = 1.5$
$\theta_1 = 0$

$\theta_0 = 0$
$\theta_1 = 0.5$

$\theta_0 = 1$
$\theta_1 = 0.5$



Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ close to y for our training examples (x,y)



$$\underset{\theta_0,\theta_1}{\text{minimize}}$$

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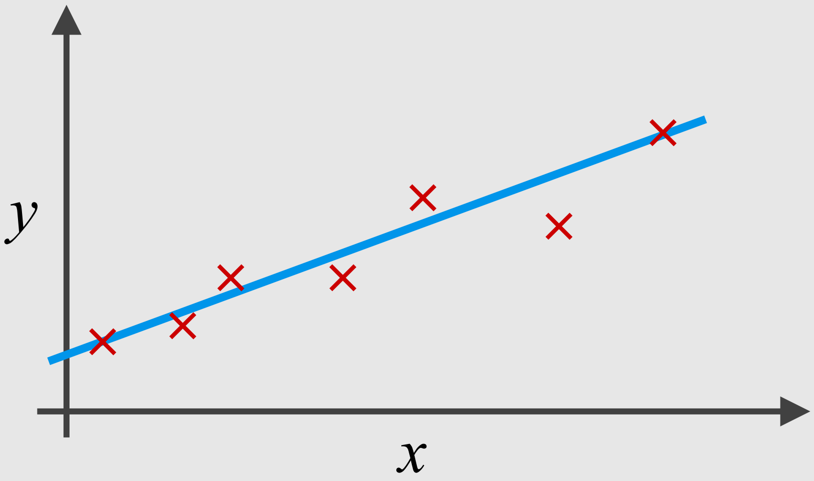
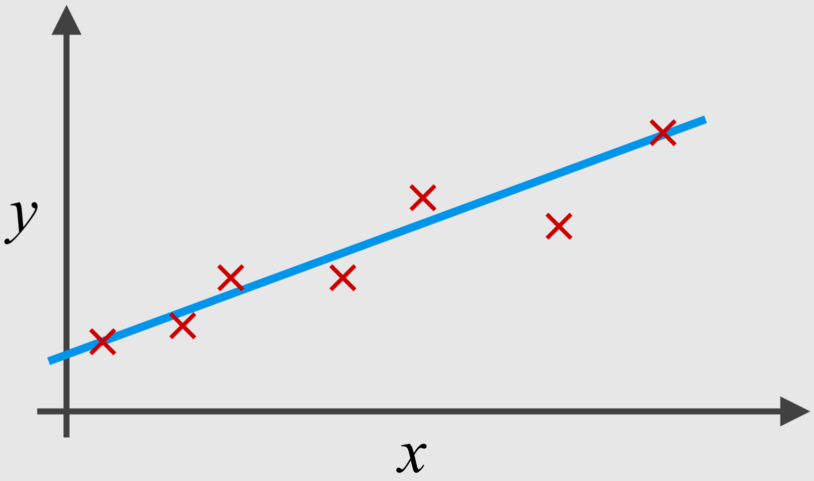


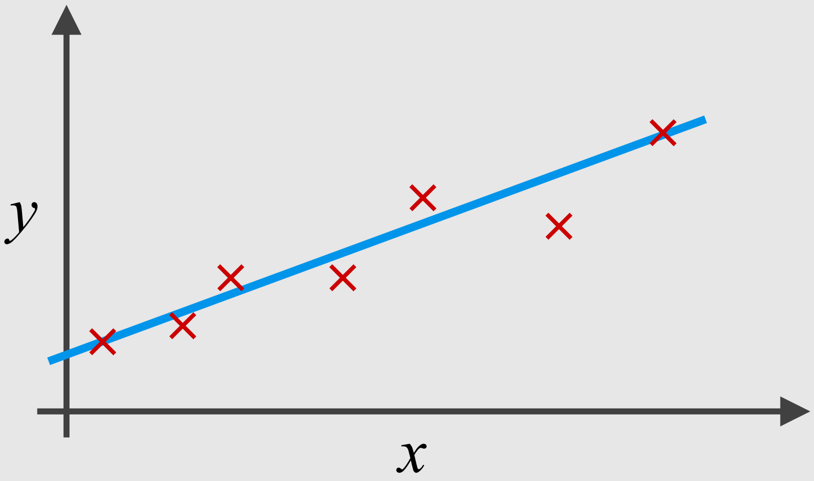
$$\underset{\theta_0,\theta_1}{\text{minimize}} \qquad (h_\theta(x \;) - y \;)^2$$

Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ close to y for our training examples (x,y)



Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ close to y for our training examples (x,y)

$$\underset{\theta_0,\theta_1}{\text{minimize}} \quad \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$



$$\underset{\theta_0,\theta_1}{\text{minimize}} \ \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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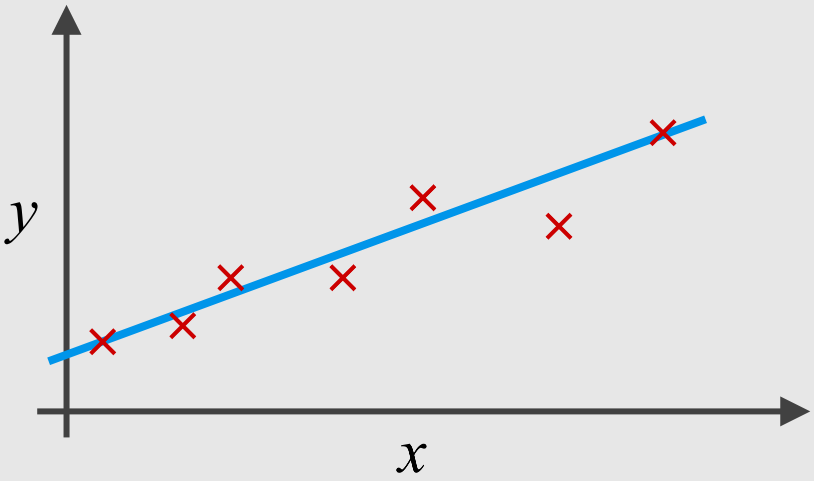
$$\underset{\theta_0,\theta_1}{\text{minimize}} \ \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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



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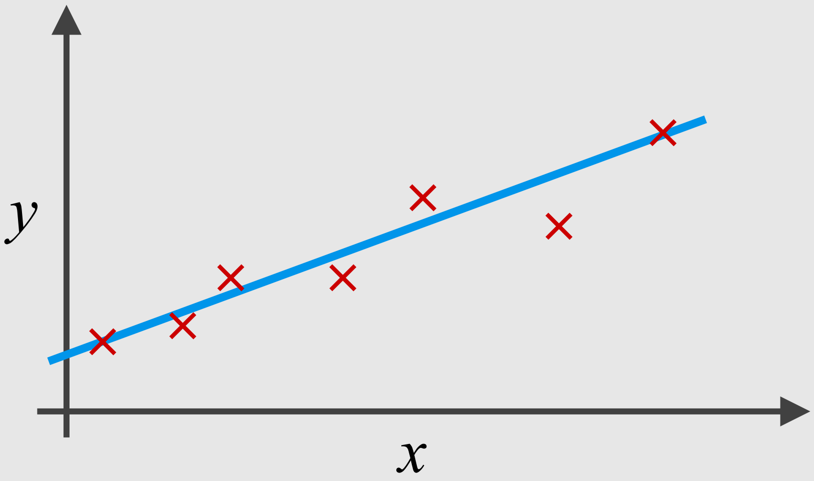

$$\underset{\theta_0,\theta_1}{\text{minimize}} \; \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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

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

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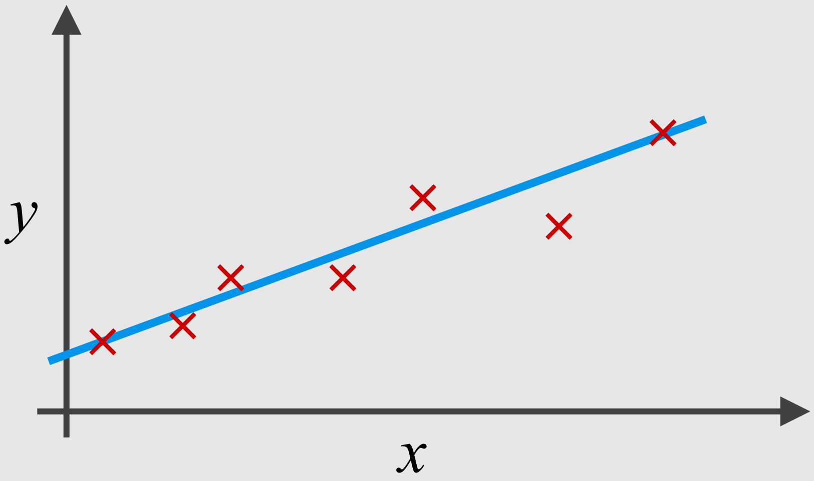

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$$J(\theta_0,\theta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$$\underset{\theta_0,\theta_1}{\text{minimize}} \ J(\theta_0,\theta_1)$$

Cost function

(Squared error function)

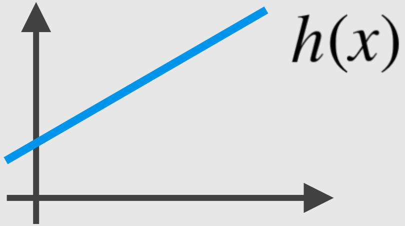
Cost Function
Intuition I

Hypothesis:

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

Parameters:

$$\theta_0, \theta_1$$



Cost Function:

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

Goal:

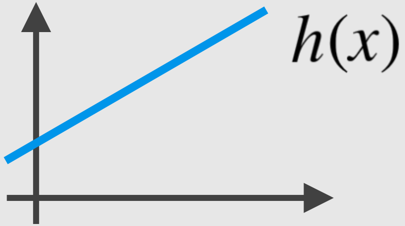
$$\underset{\theta_0,\theta_1}{\text{minimize}}\ J(\theta_0,\theta_1)$$

Hypothesis:

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

Parameters:

$$\theta_0, \theta_1$$



Cost Function:

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

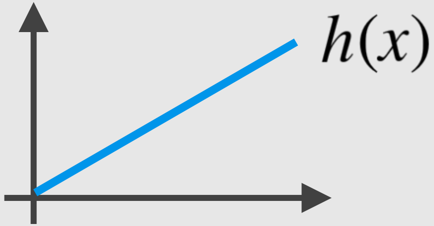
Goal:

$$\underset{\theta_0,\theta_1}{\text{minimize}}\ J(\theta_0,\theta_1)$$

<u>Simplified</u>

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

$$\theta_1$$



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

$$\underset{\theta_1}{\text{minimize}}\ J(\theta_1)$$

$h_\theta(x)$

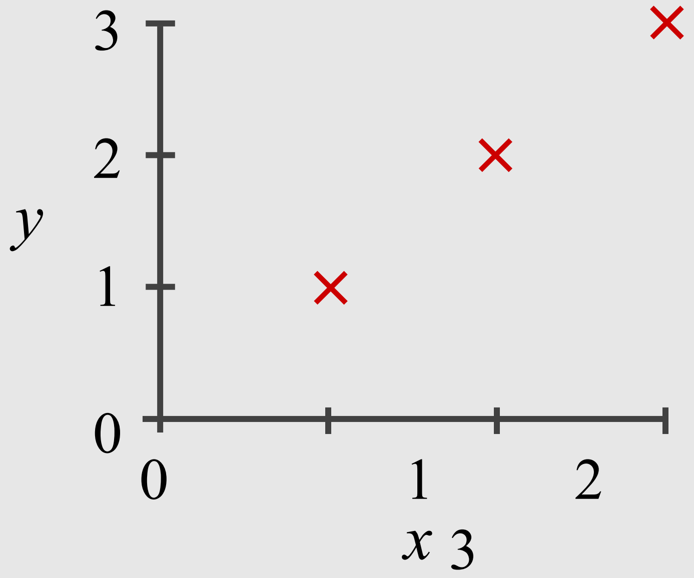
(for fixed θ_1 , this is a function of x)

$J(\theta_1)$

(function of the parameters θ_1)

$h_\theta(x)$

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

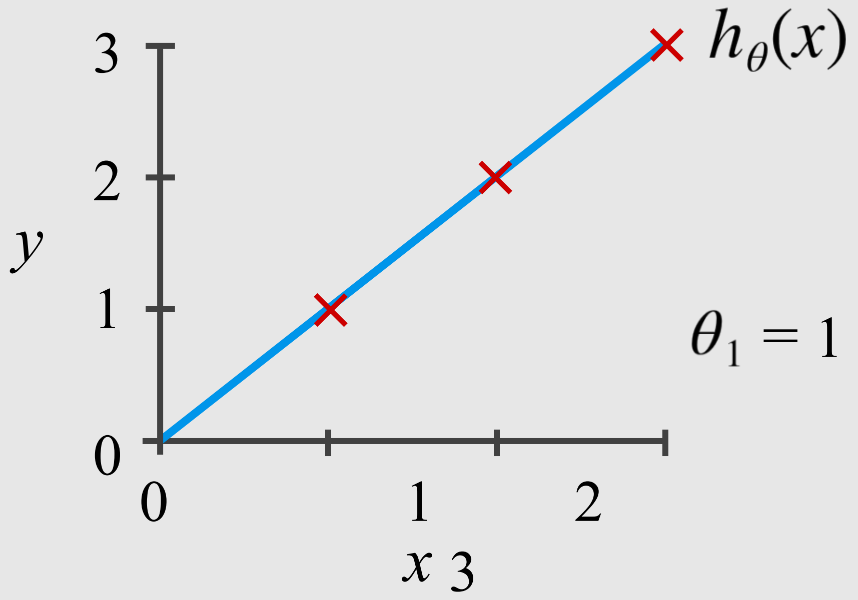


$J(\theta_1)$

(function of the parameters θ_1)

$h_\theta(x)$

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



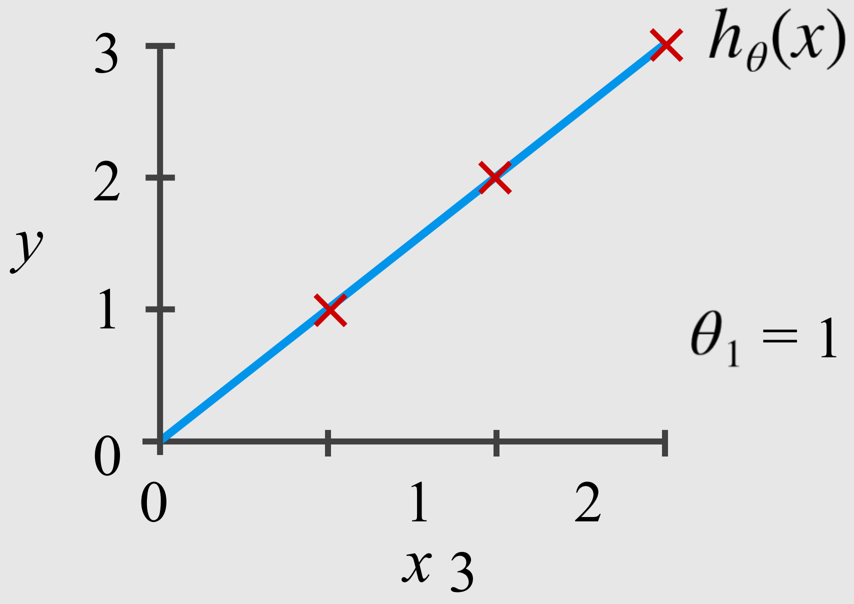
$J(\theta_1) = J(1) = ?$

$J(\theta_1)$

(function of the parameters θ_1)

$h_\theta(x)$

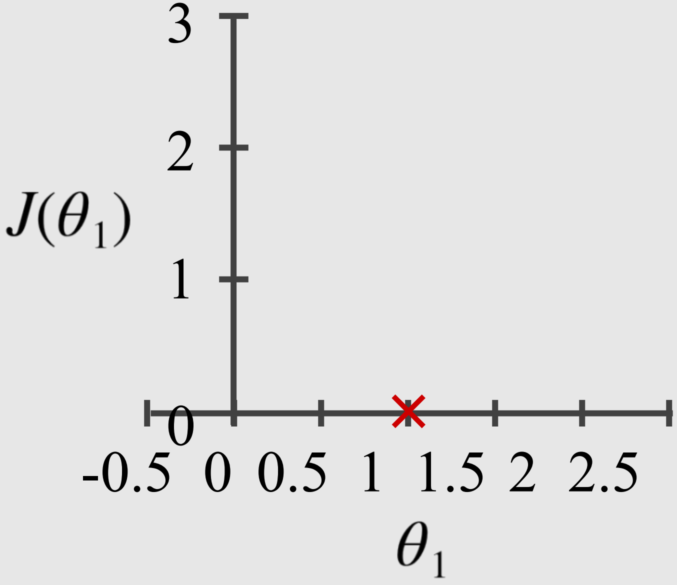
(for fixed θ_1 , this is a function of x)



$J(\theta_1) = J(1) = 0$

$J(\theta_1)$

(function of the parameters θ_1)



$h_\theta(x)$

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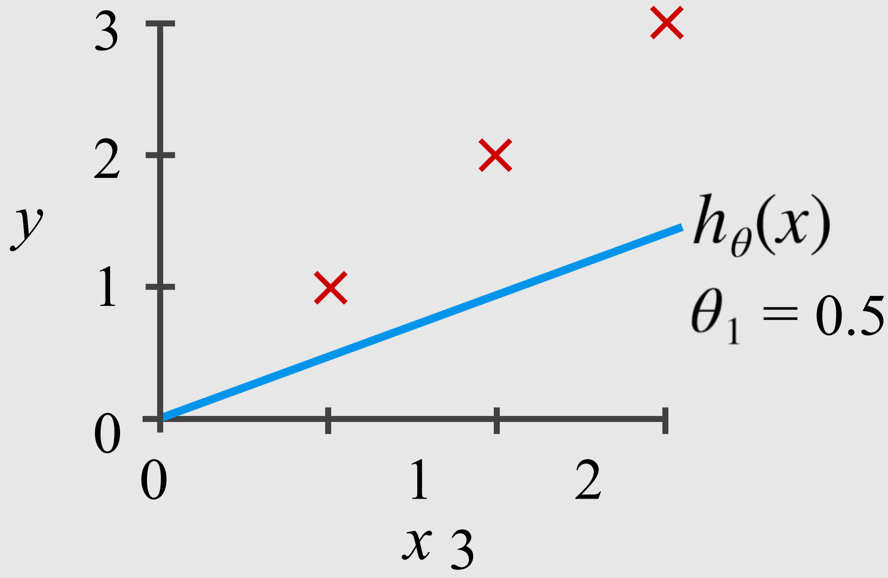
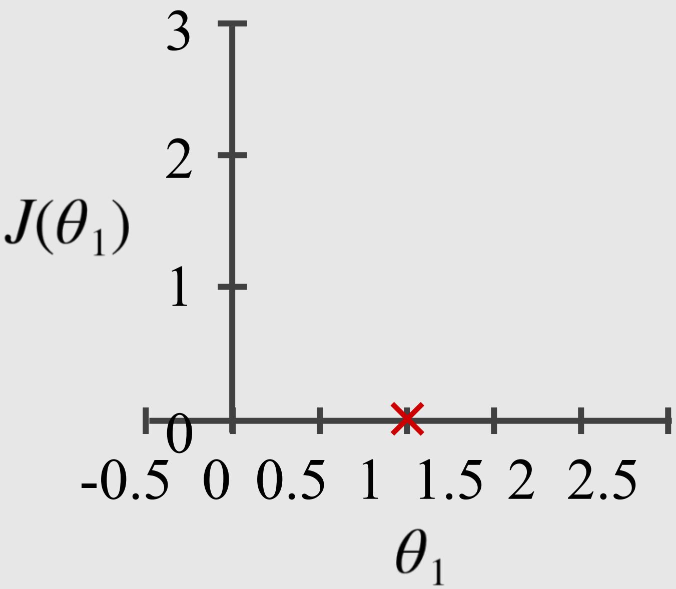


$J(\theta_1)$

(function of the parameters θ_1)



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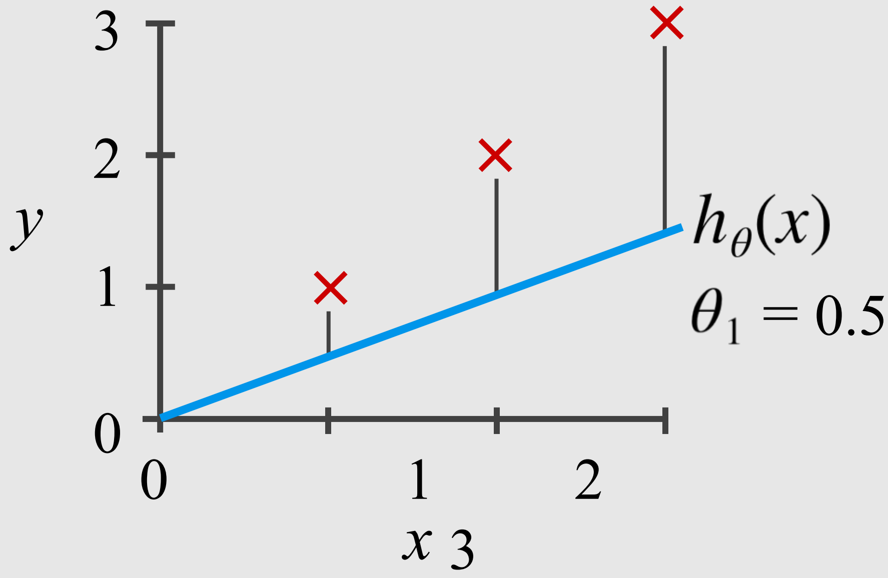
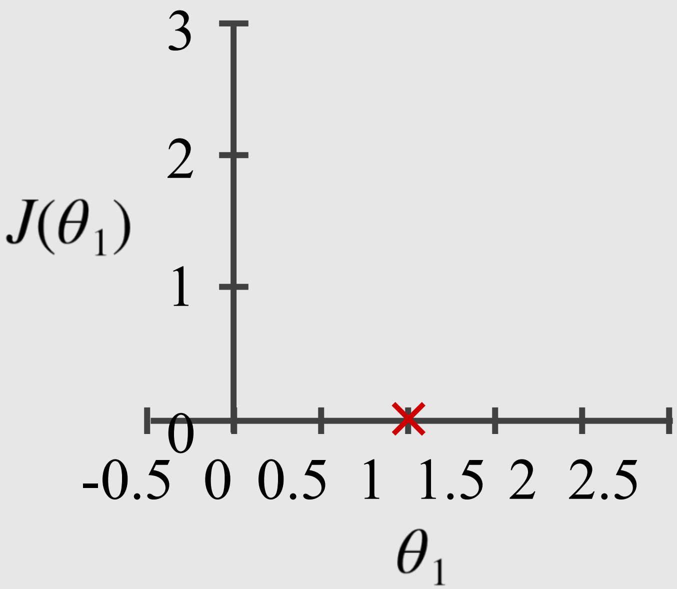


$J(\theta_1)$

(function of the parameters θ_1)



$h_\theta(x)$

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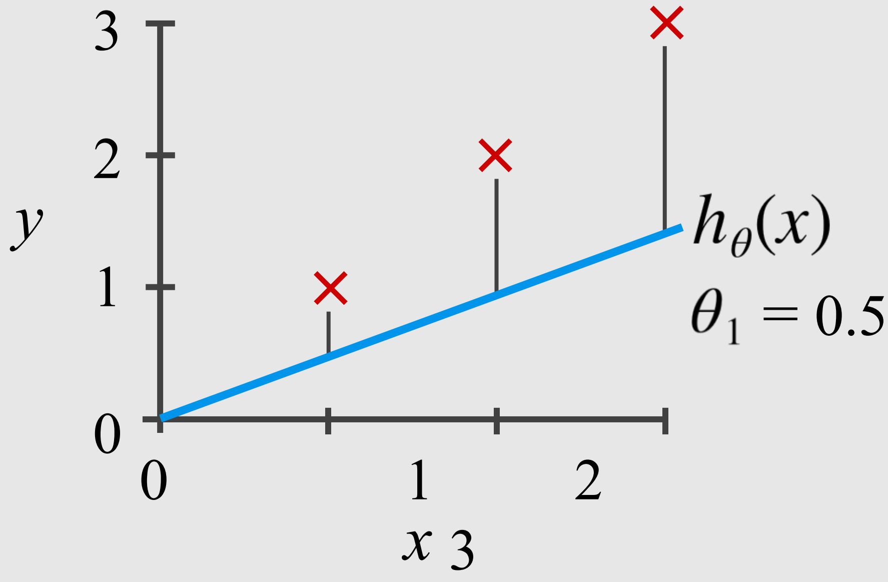
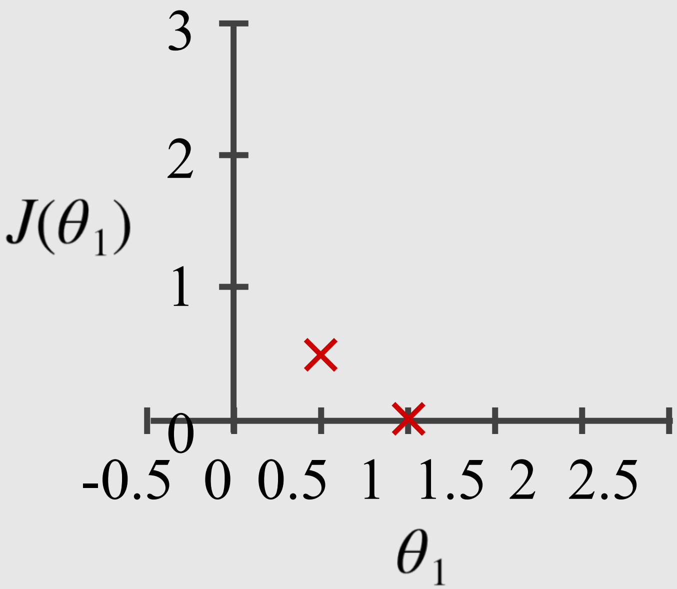


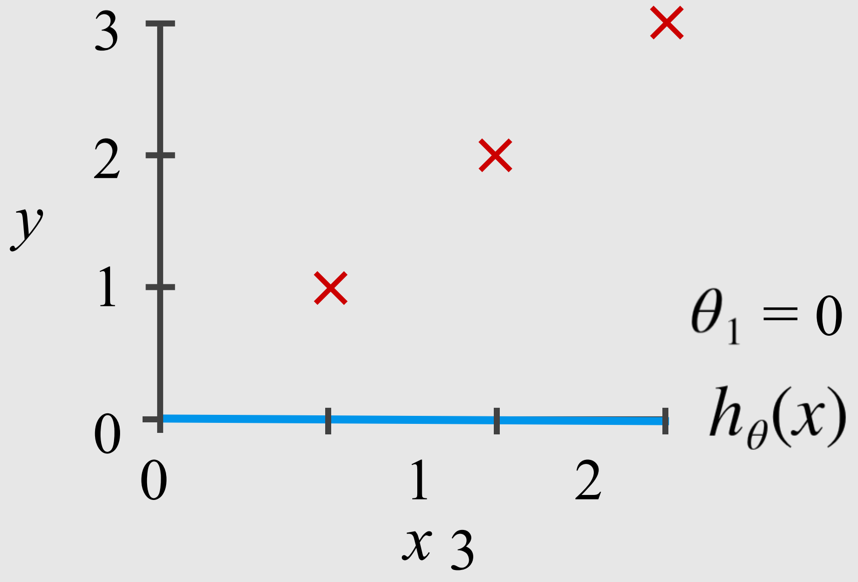
$J(\theta_1)$

(function of the parameters θ_1)



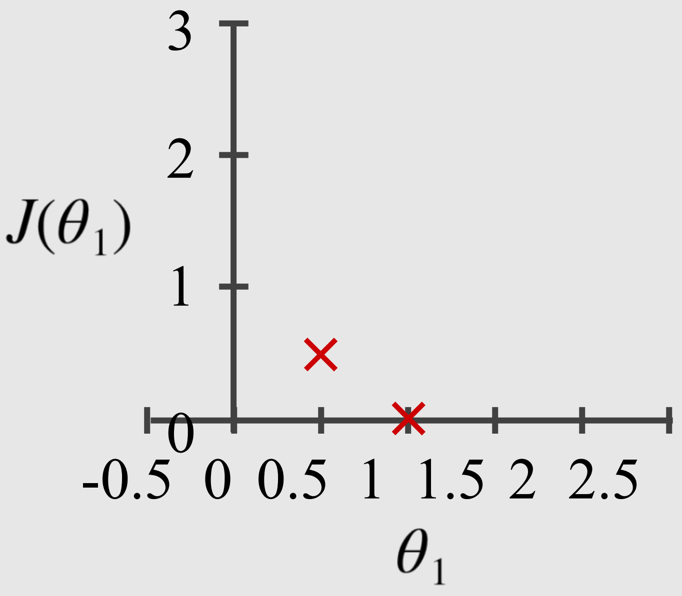
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameters θ_1)



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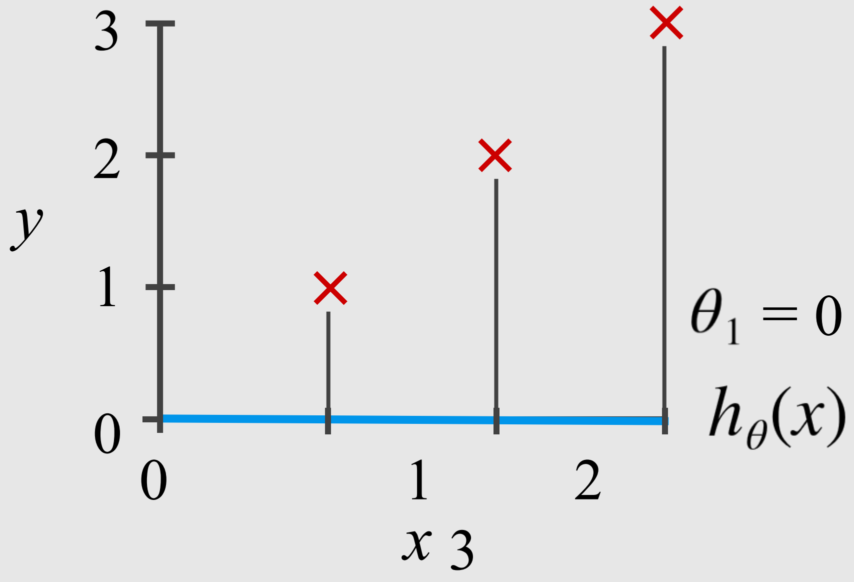
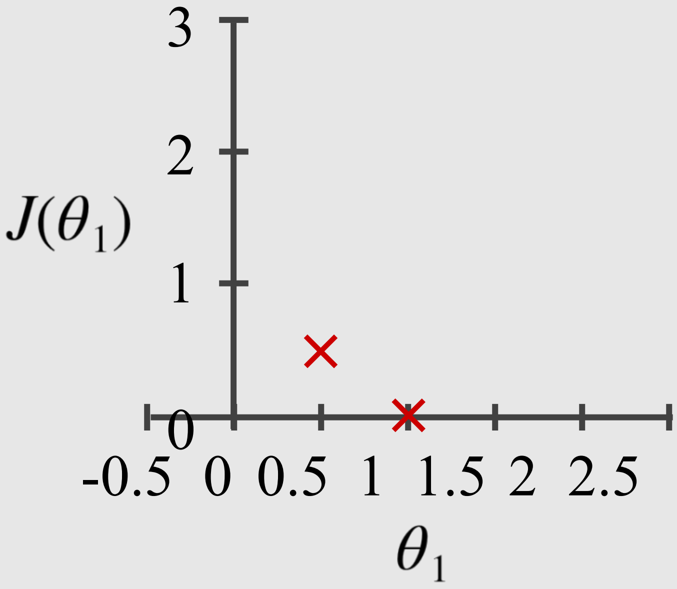


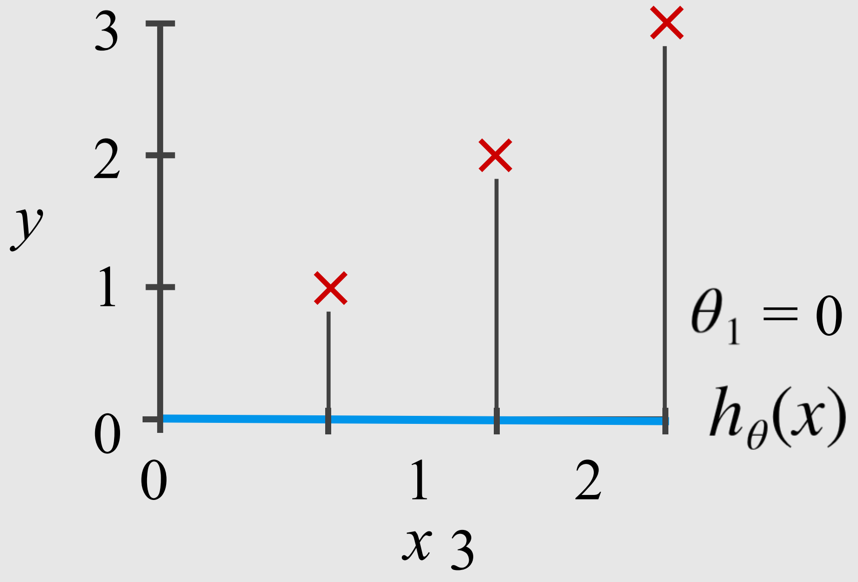
$J(\theta_1)$

(function of the parameters θ_1)



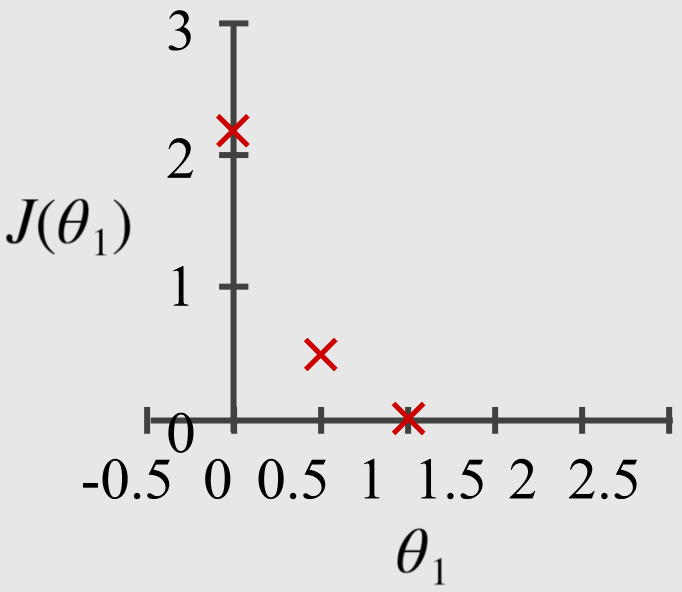
$h_\theta(x)$

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



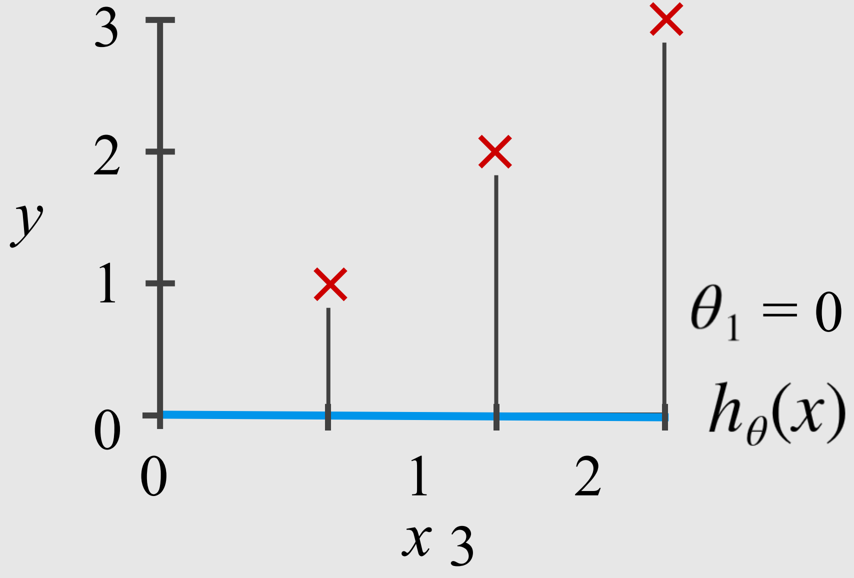
$J(\theta_1)$

(function of the parameters θ_1)



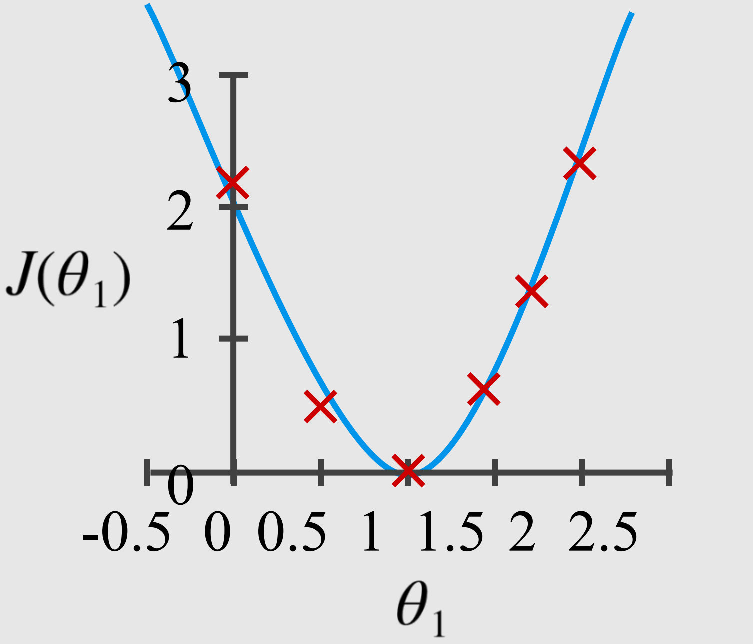
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameters θ_1)



Cost Function

Intuition II

$h_\theta(x)$

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

$J(\theta_0, \theta_1)$

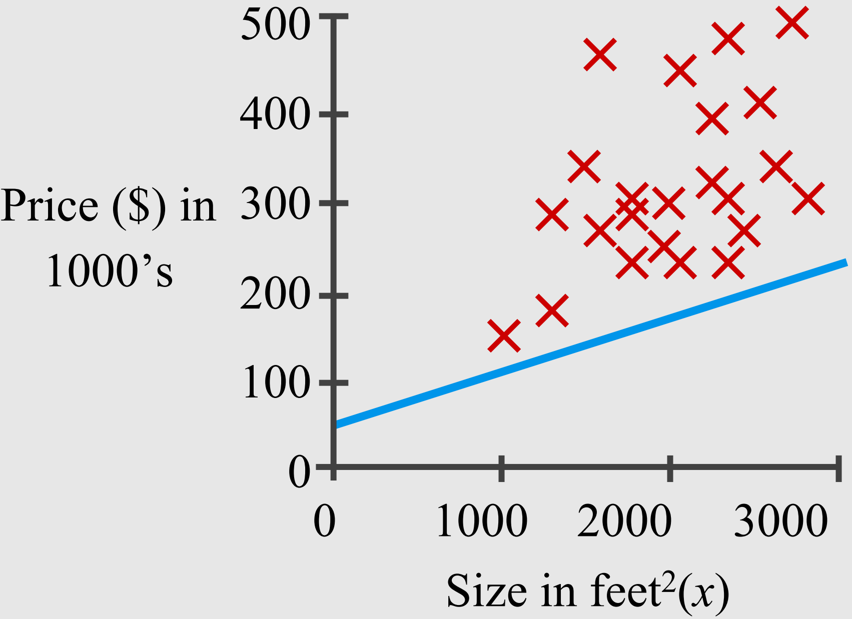
(function of the parameters θ_0, θ_1)

$h_\theta(x)$

(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)



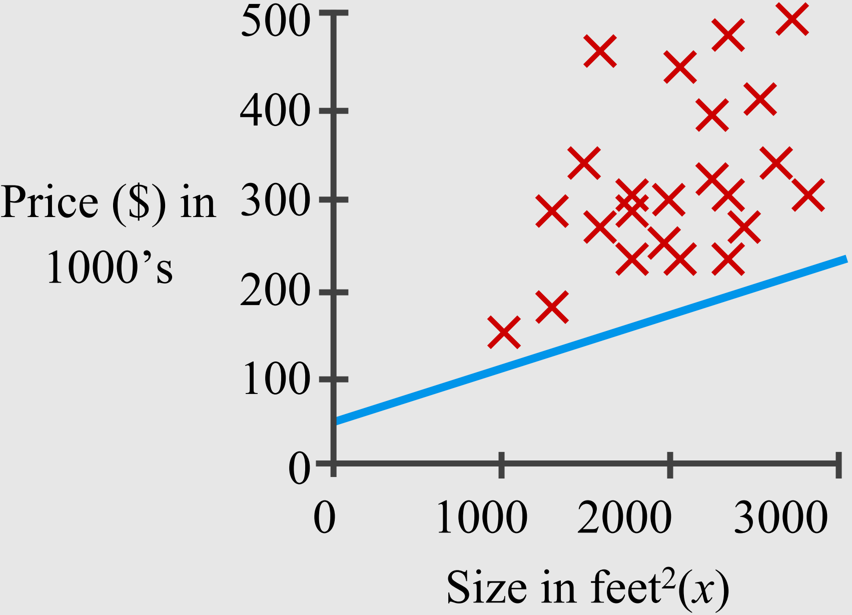
$$h_\theta(x) = 50 + 0.06x$$

$\theta_0 = 50$

$\theta_1 = 0.06$

$h_\theta(x)$

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



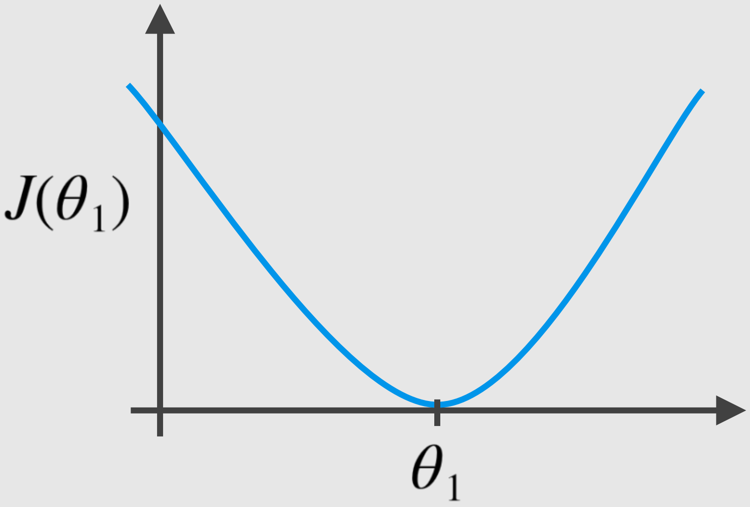
$h_\theta(x) = 50 + 0.06x$

$\theta_0 = 50$

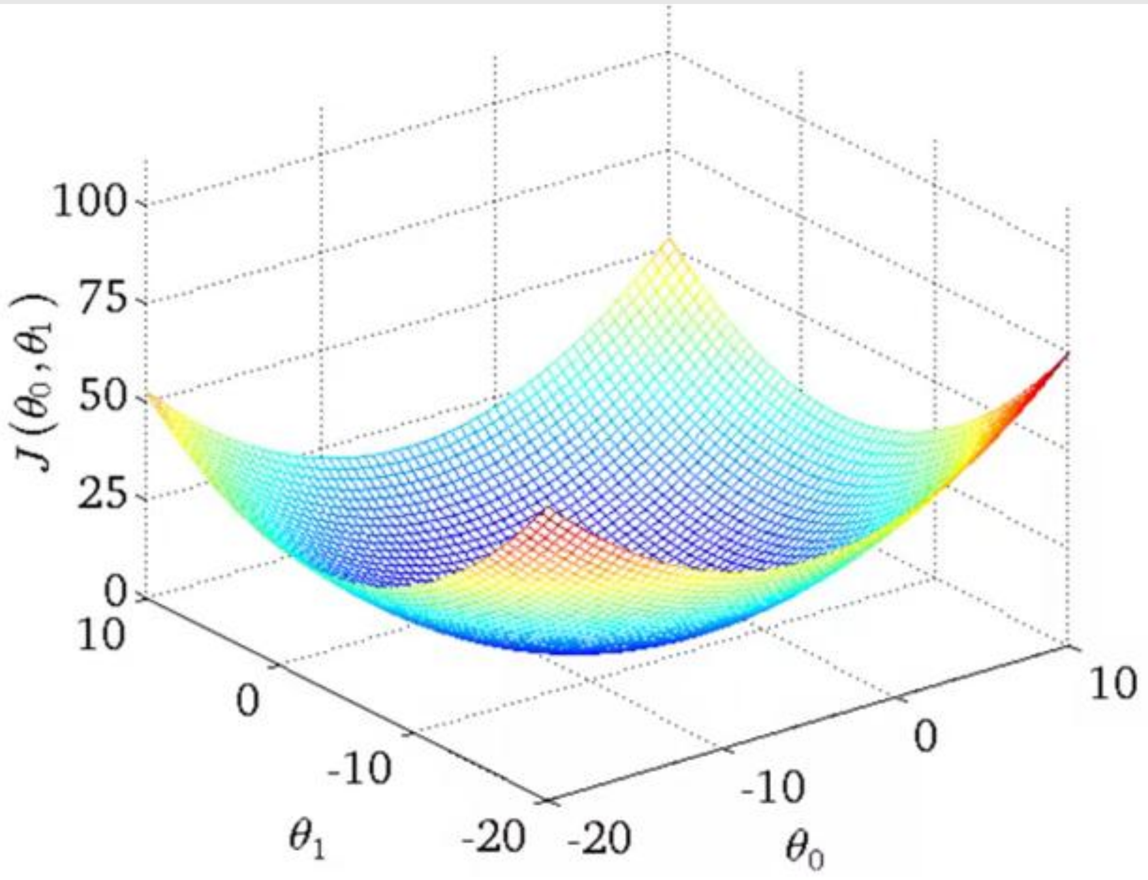
$\theta_1 = 0.06$

$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

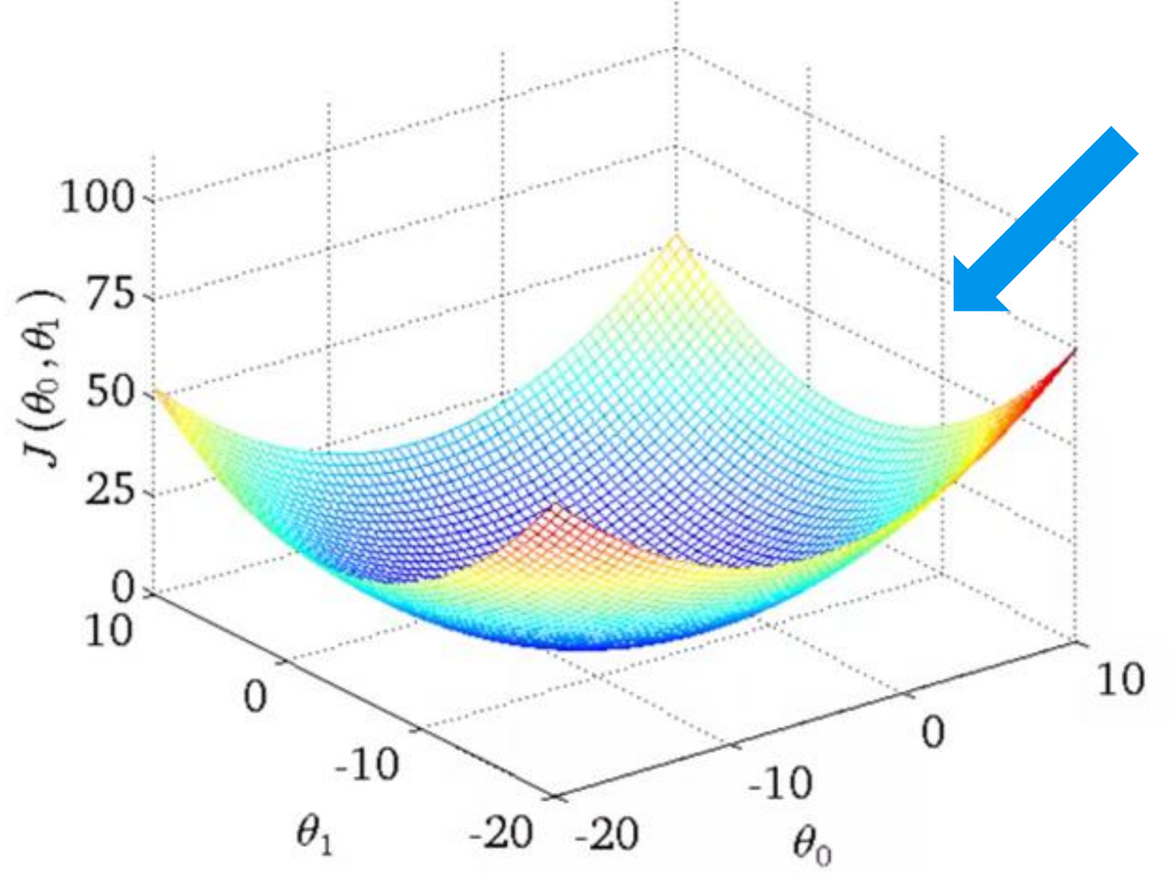


θ_0 and θ_1?



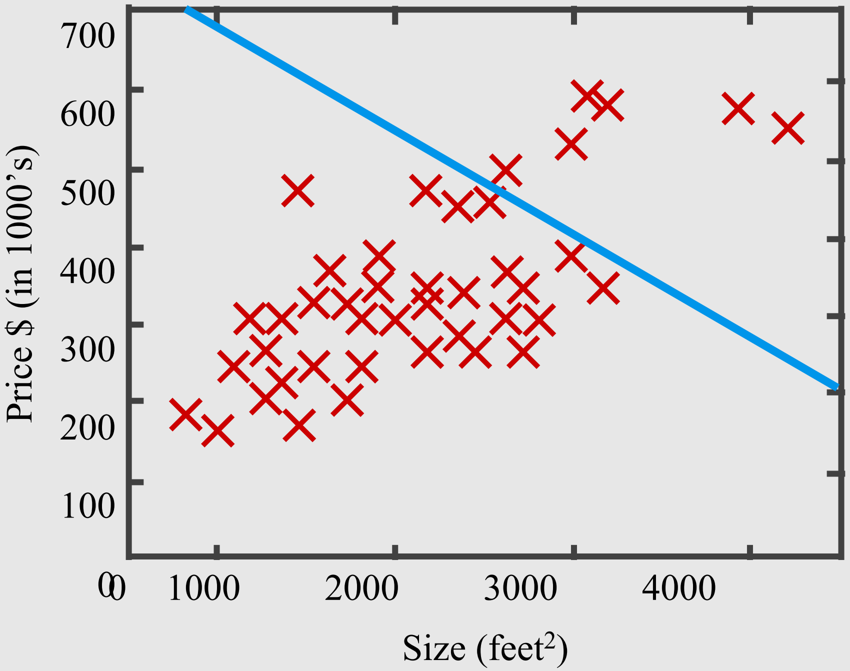
100
75
50
25
0
$J(\theta_0, \theta_1)$
10
0
-10
-20
θ_1
-20
-10
0
10
θ_0

Convex Function



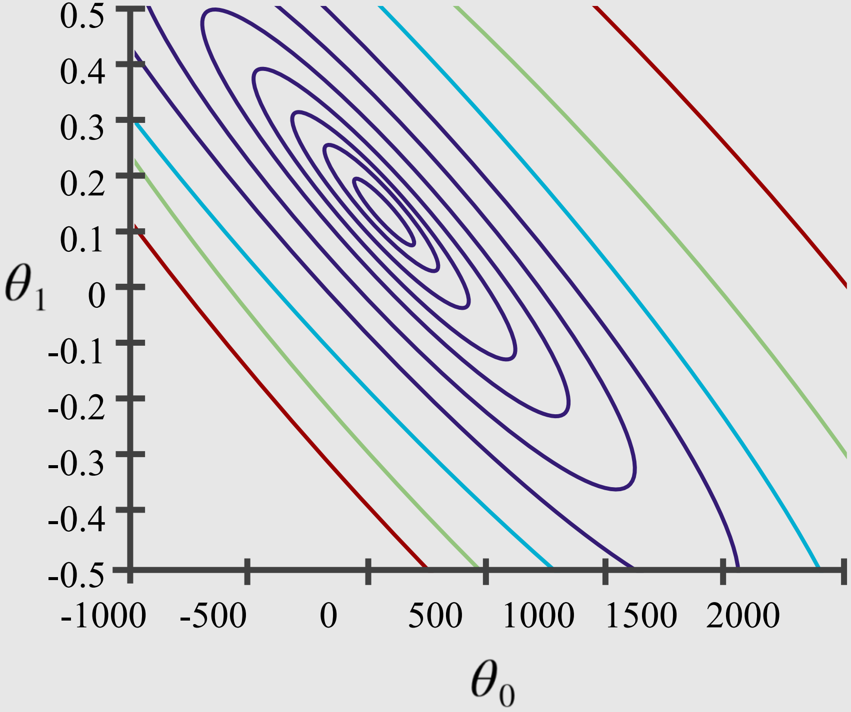
$h_\theta(x)$

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



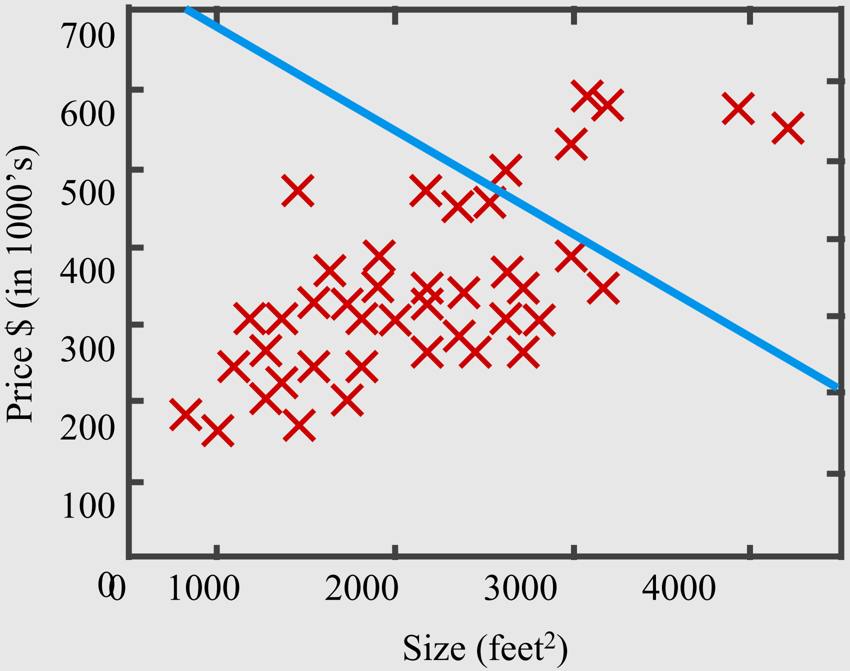
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



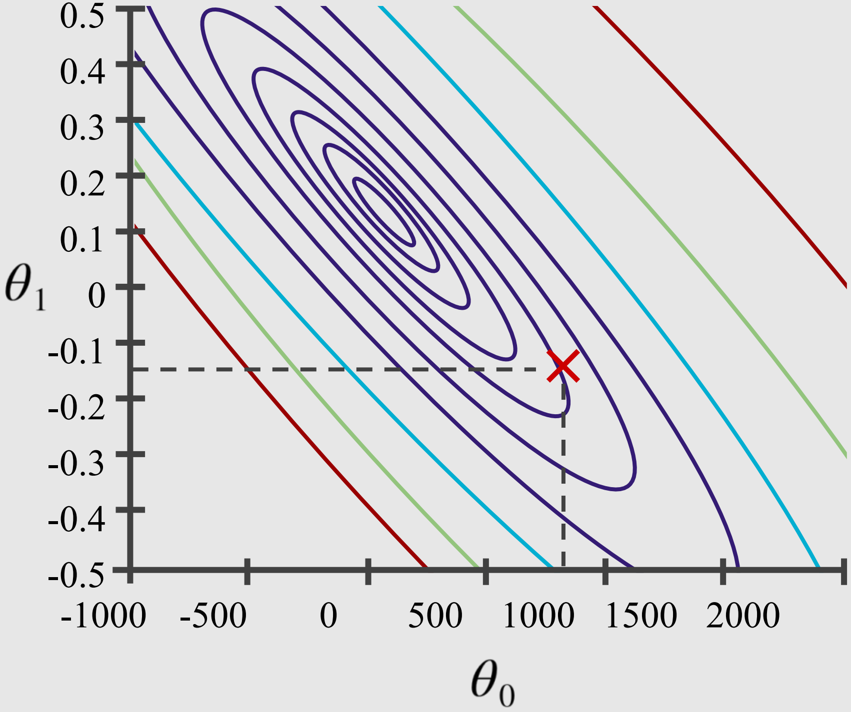
$h_\theta(x)$

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



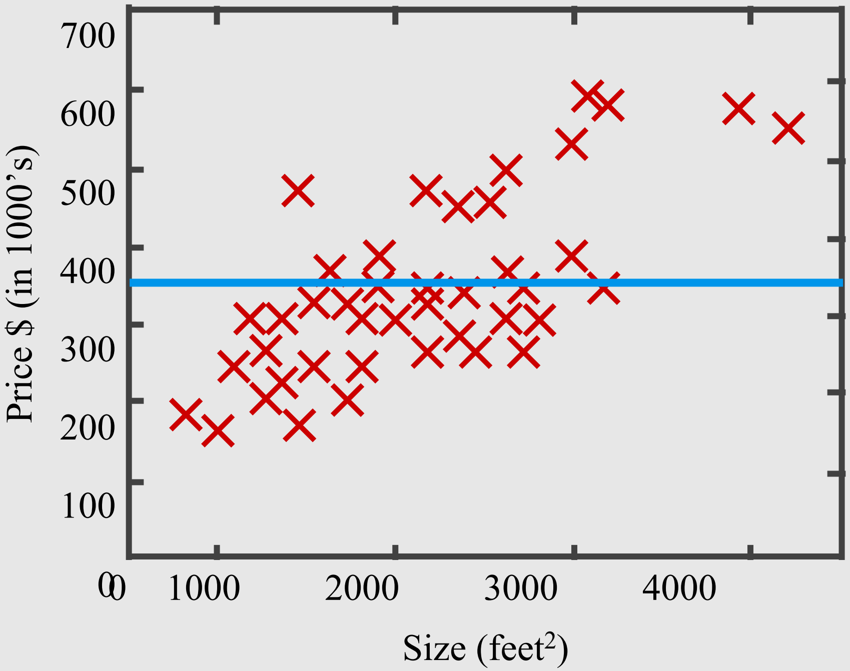
$J(\theta_0,\theta_1)$

(function of the parameters θ_0, θ_1)



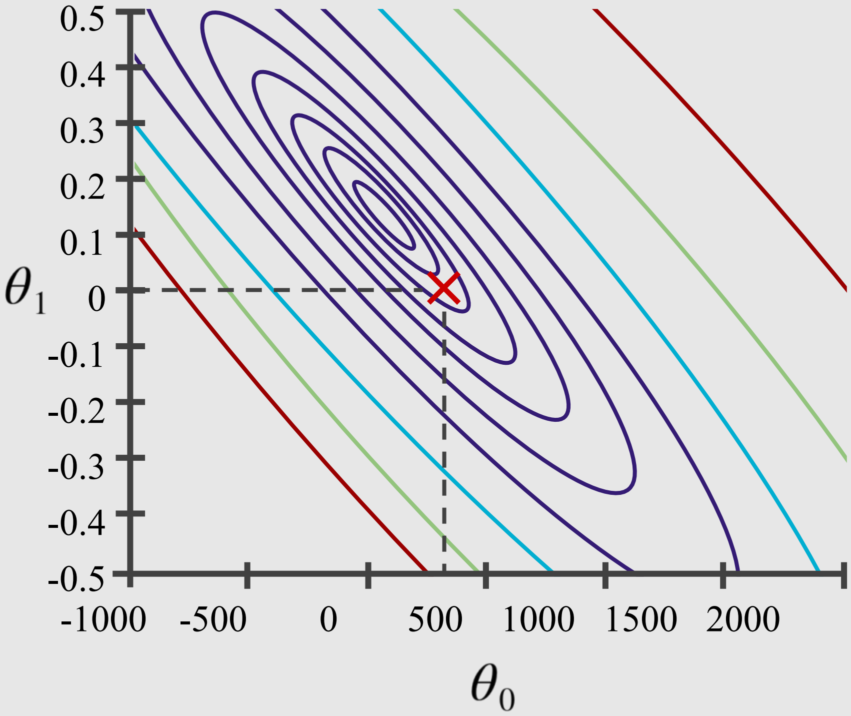
$h_\theta(x)$

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



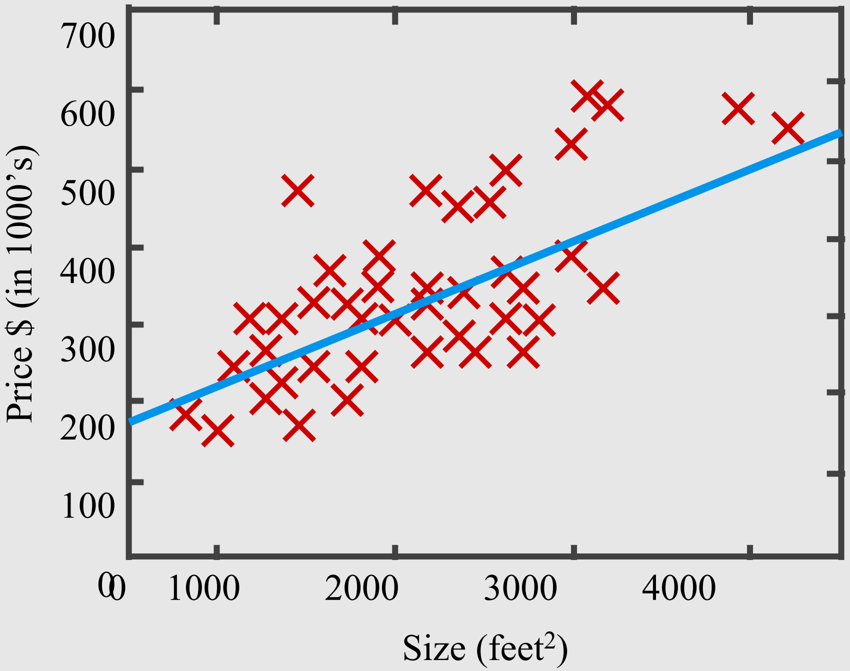
$J(\theta_0,\theta_1)$

(function of the parameters θ_0, θ_1)



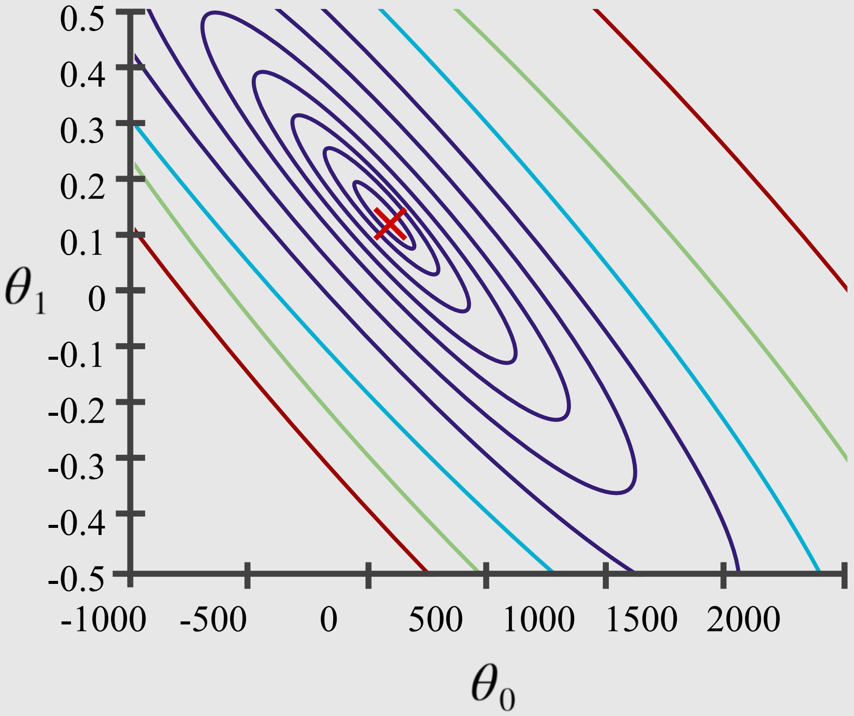
$h_\theta(x)$

(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)



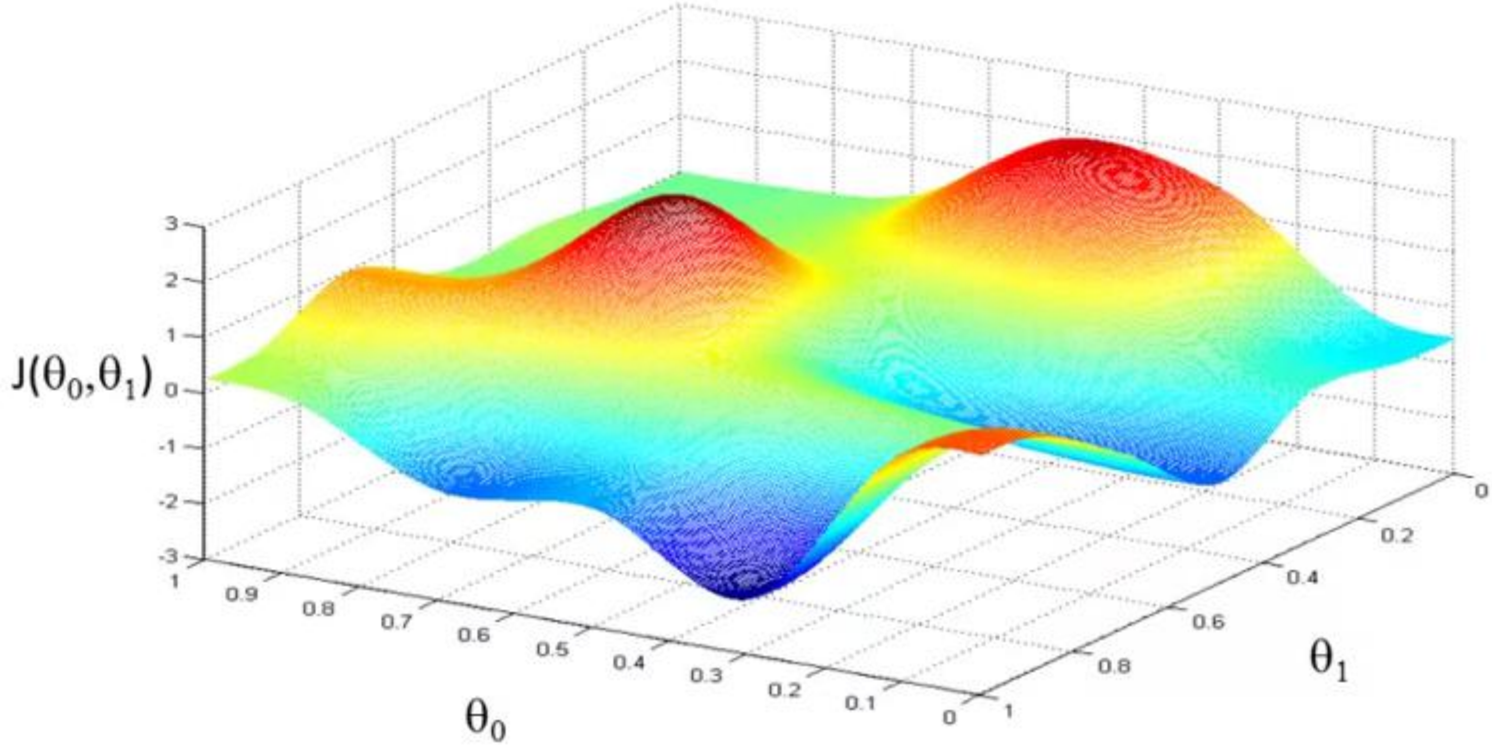
Gradient Descent

Have some function $J(\theta_0,\theta_1)$

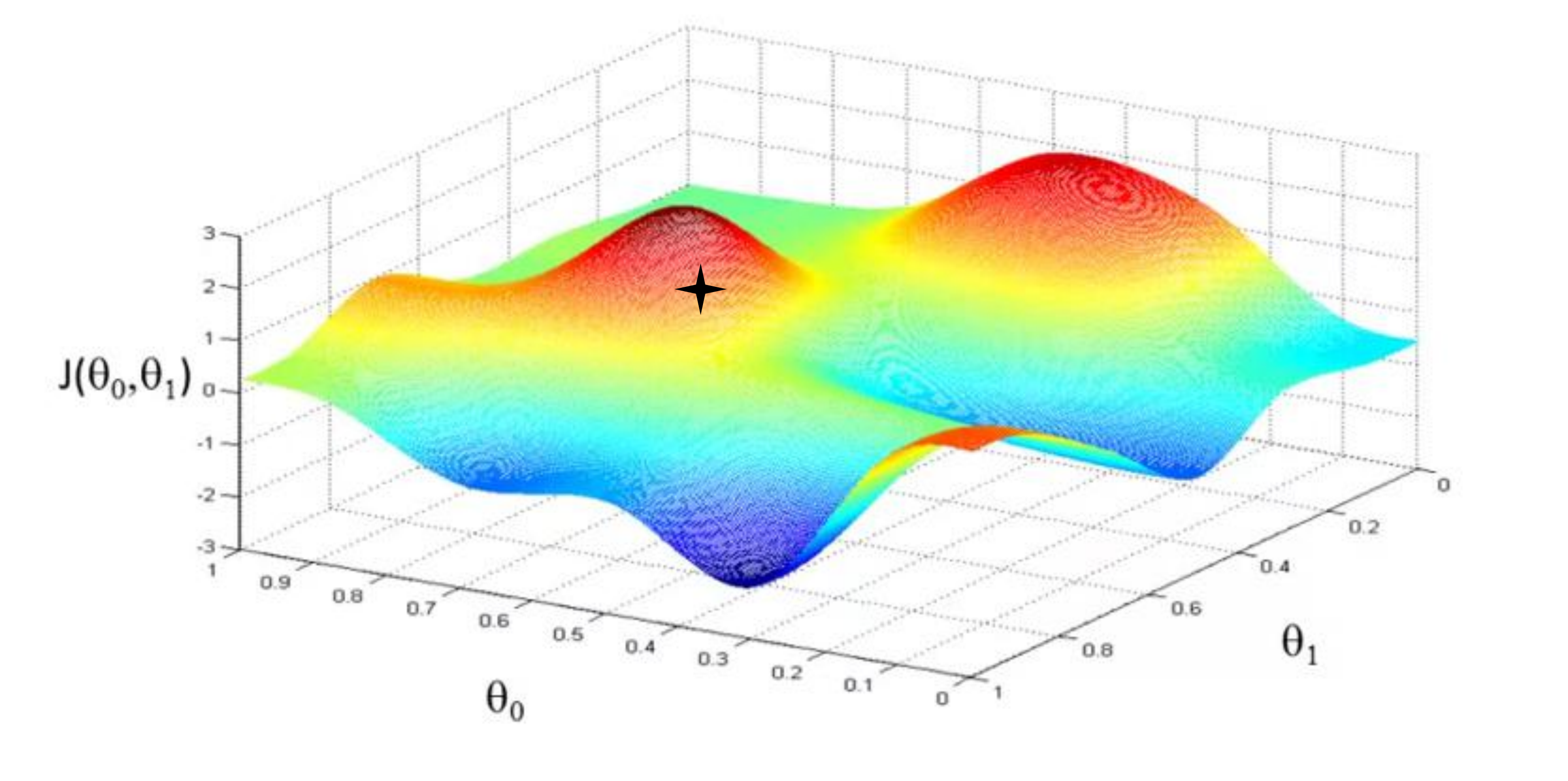
Want $\underset{\theta_0,\theta_1}{\text{minimize}}\, J(\theta_0,\theta_1)$

Outline:

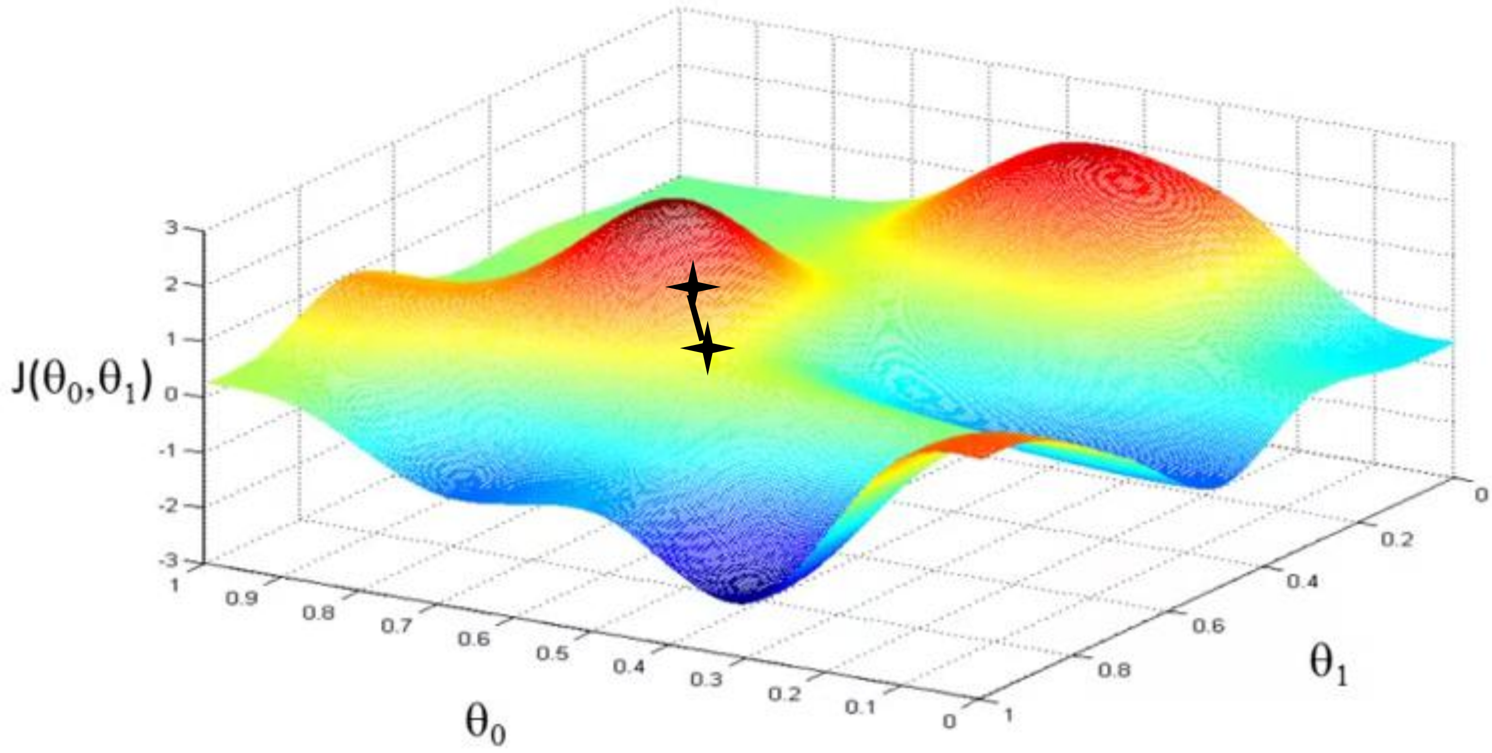
- Start with some θ_0, θ_1
- Keep changing θ_0, θ_1 to reduce $J(\theta_0,\theta_1)$ until we hopefully end up at a minimum



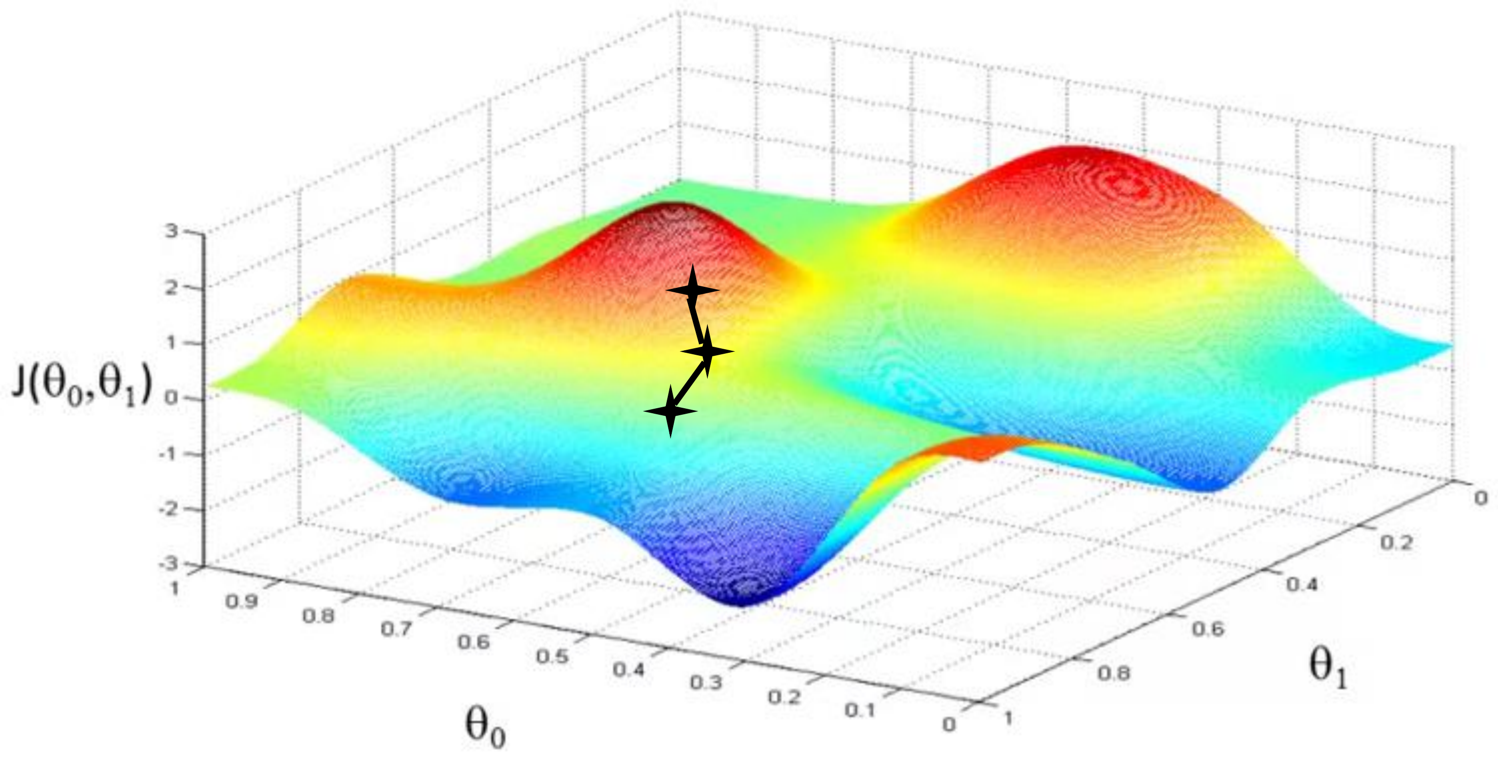
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
θ_0
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_1
0
0.2
0.4
0.6
0.8
1



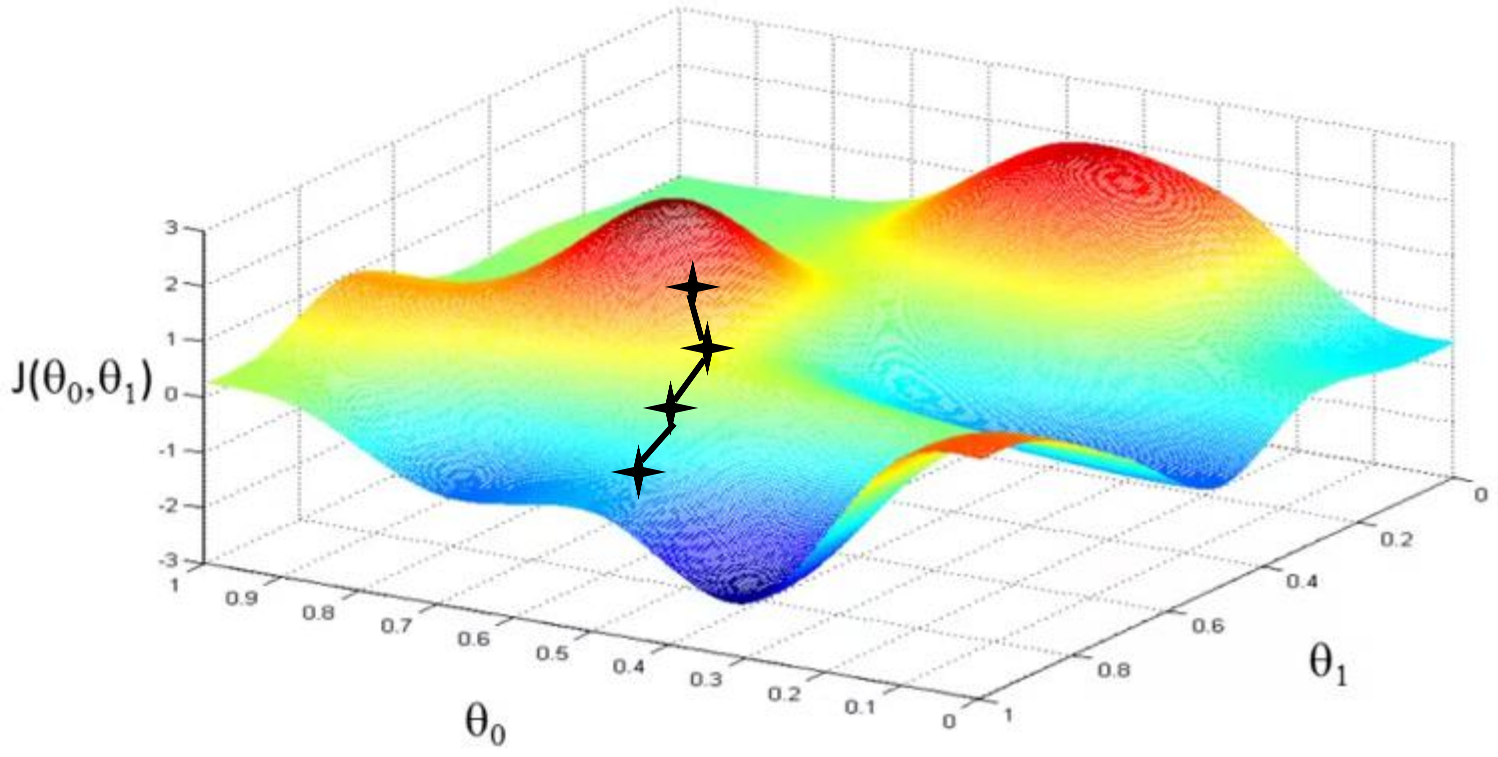
J(θ0,θ1)
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1



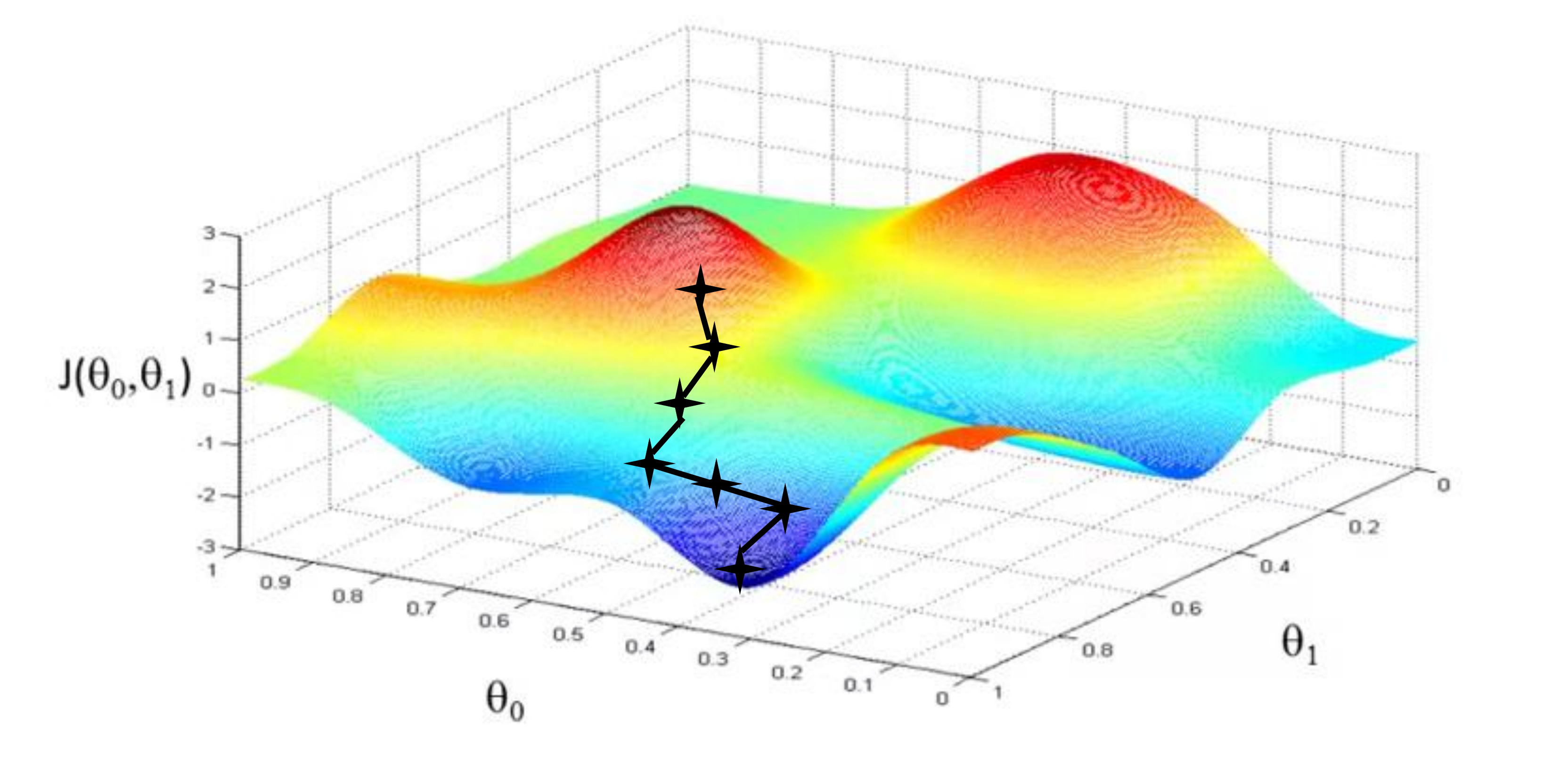
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
θ_0
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_1
0
0.2
0.4
0.6
0.8
1



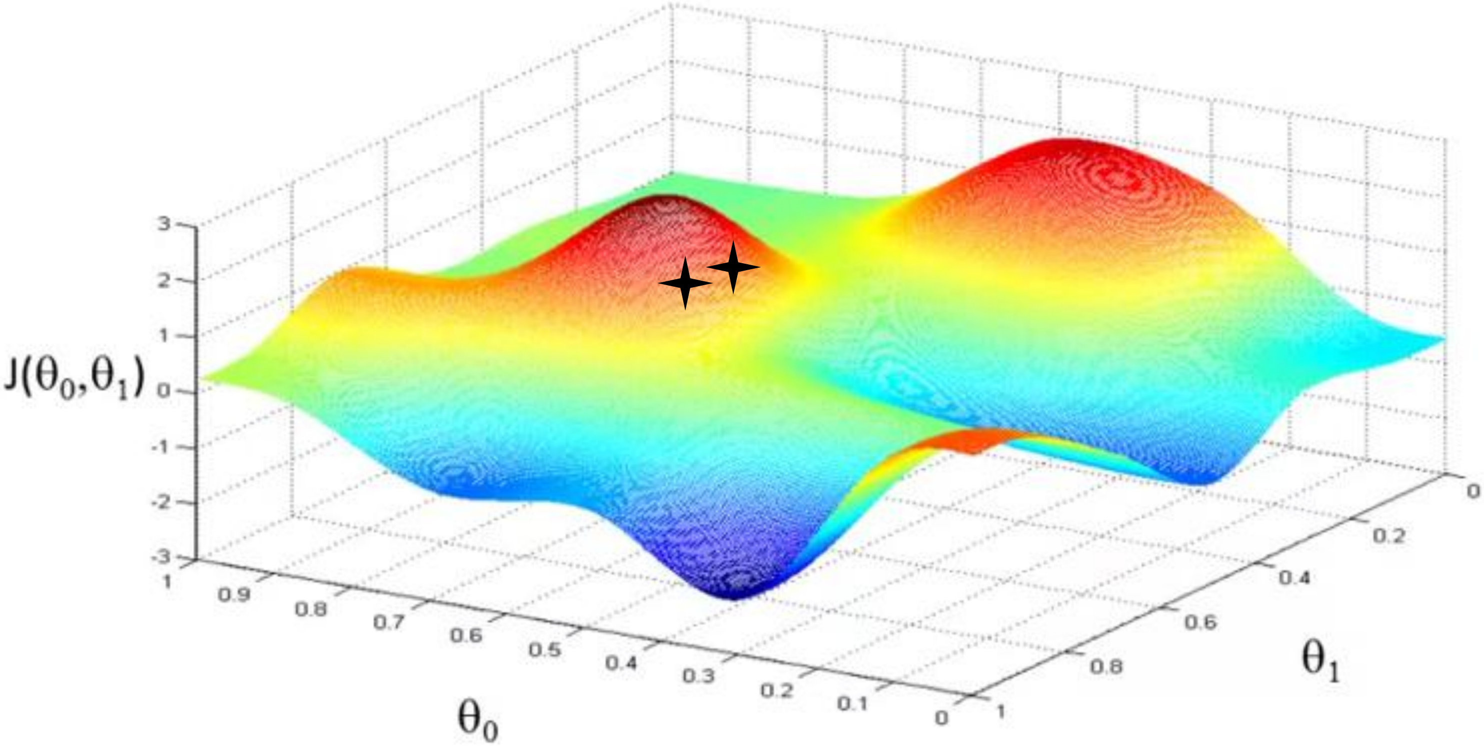
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



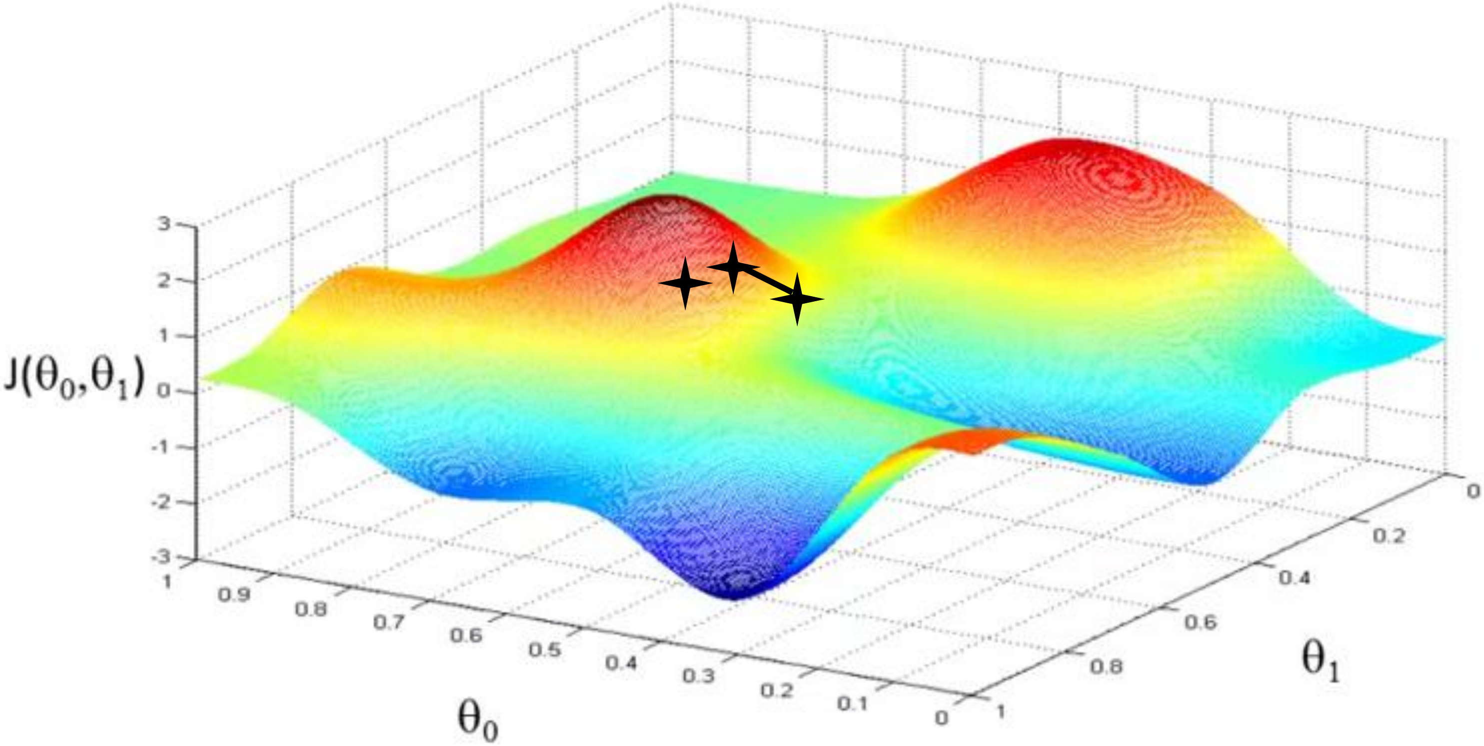
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



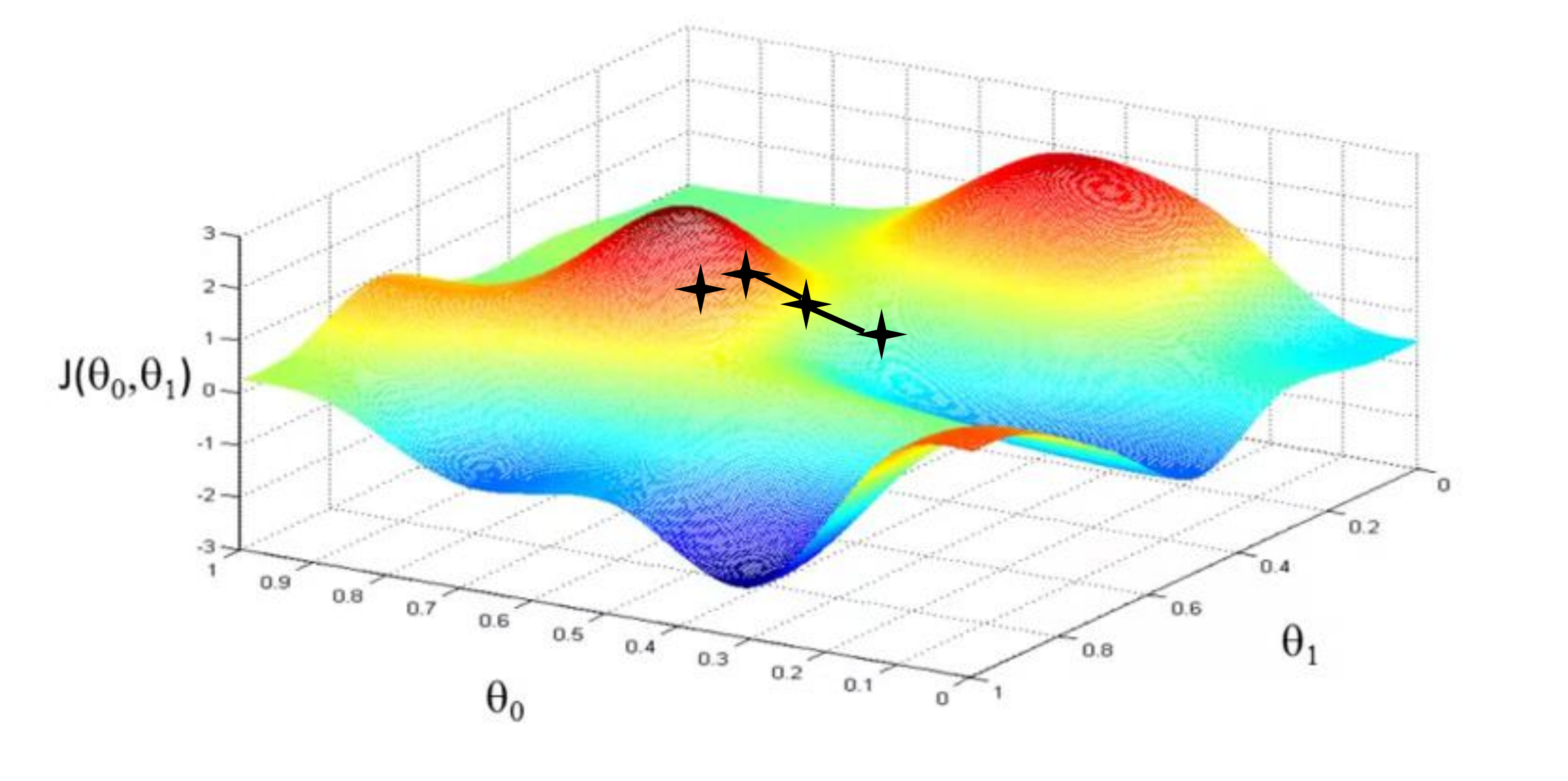
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



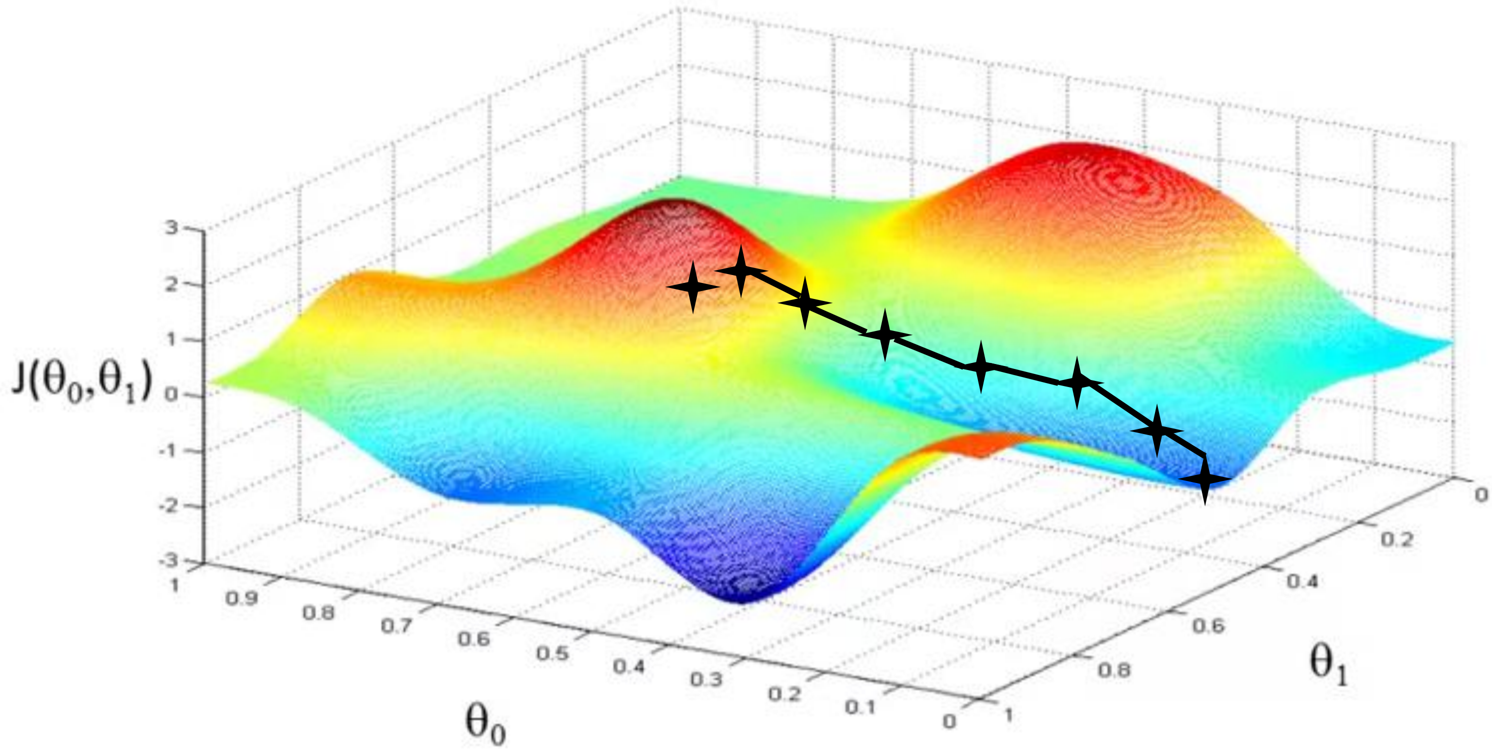
$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1



$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1

Gradient Descent algorithm

repeat until convergence {

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

}

(simultaneously update

$j = 0$ and $j = 1$)

Gradient Descent algorithm

repeat until convergence {

$$\theta_j := \theta_j - \alpha \boxed{\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)}$$

}

(simultaneously update

$j = 0$ and $j = 1$)

Learning rate

Derivative term

Gradient Descent algorithm

repeat until convergence {

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

}

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

repeat until convergence {

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

}

Correct: Simultaneous update

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

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

$$\theta_0 := \text{temp0}$$

$$\theta_1 := \text{temp1}$$

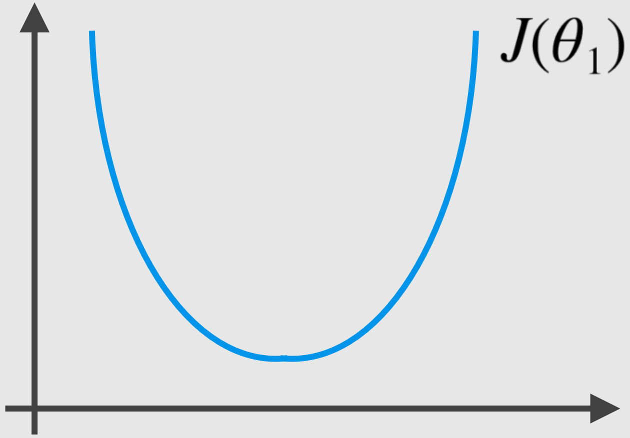
Incorrect

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

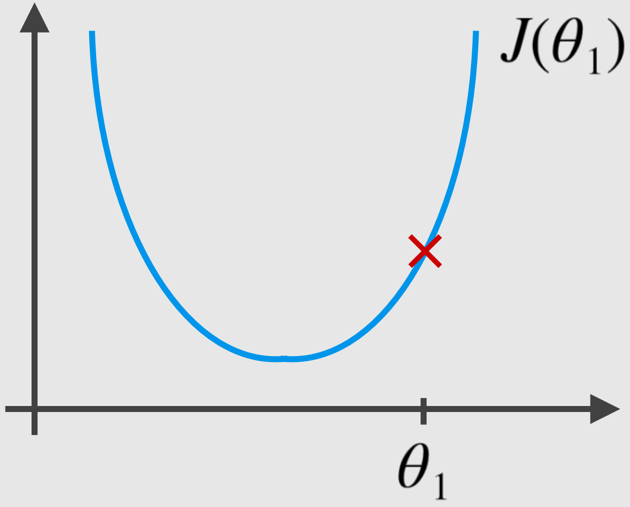
$$\theta_0 := \text{temp0}$$

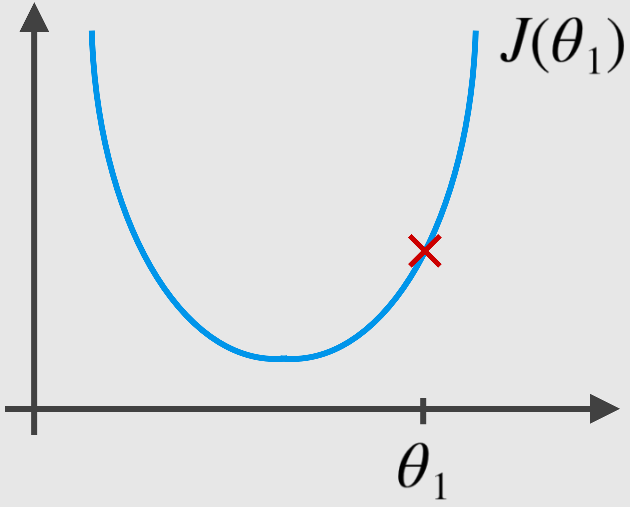
$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_1 := \text{temp1}$$


$J(\theta_1)$

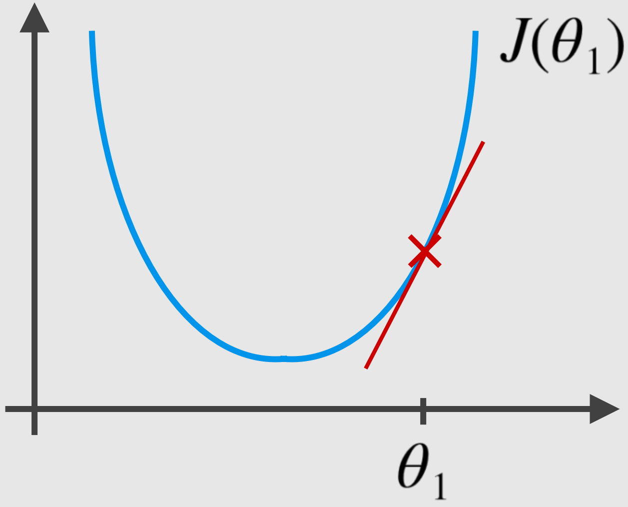
$$\theta_1 \in \mathbb{R}$$





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

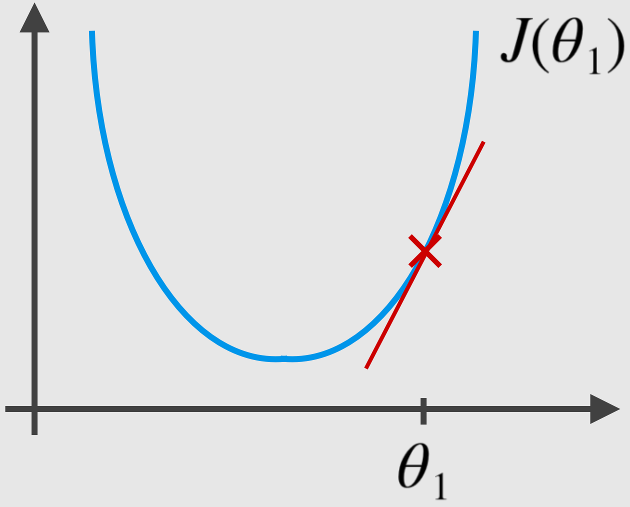
$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$



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

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

$\theta_1 \in \mathbb{R}$

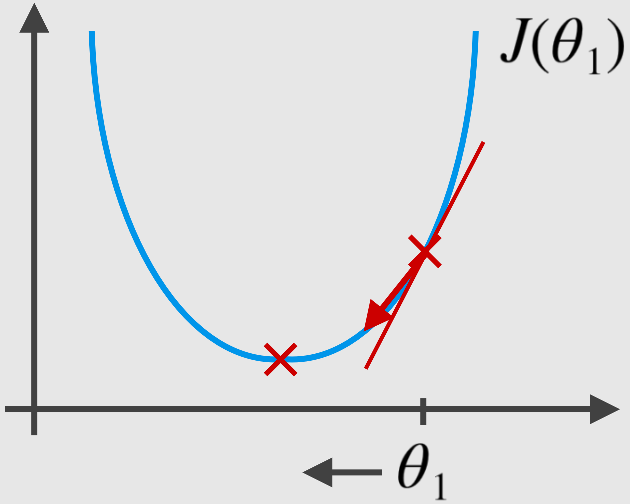


$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$

≥ 0

$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$

$\theta_1 \in \mathbb{R}$

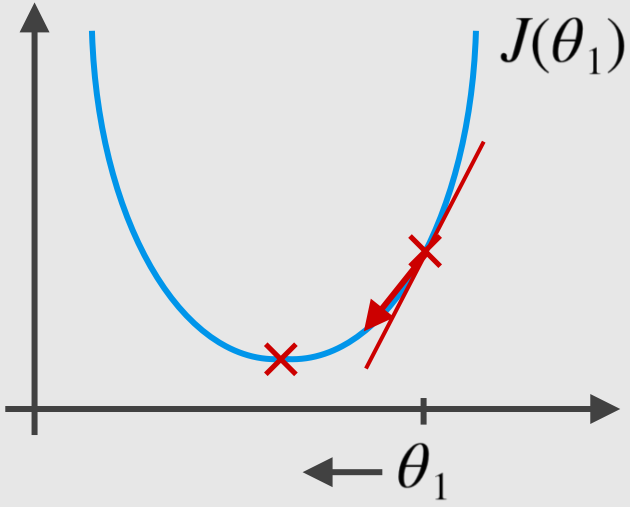


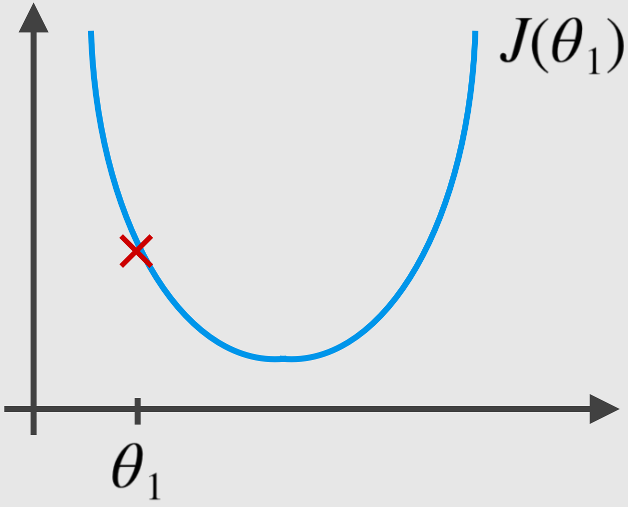
$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$

≥ 0

$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$

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

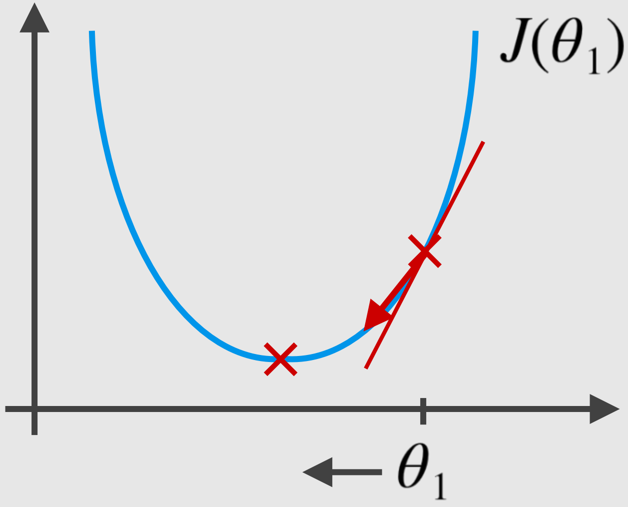




$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)} \quad \geq 0$$

$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$

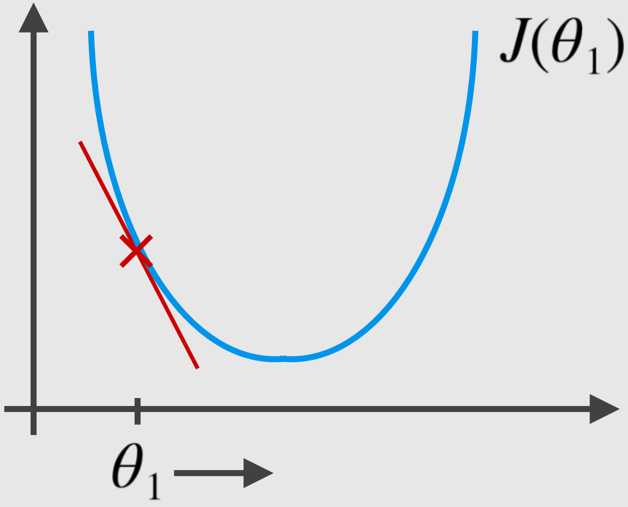
$\theta_1 \in \mathbb{R}$



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

≥ 0

$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$

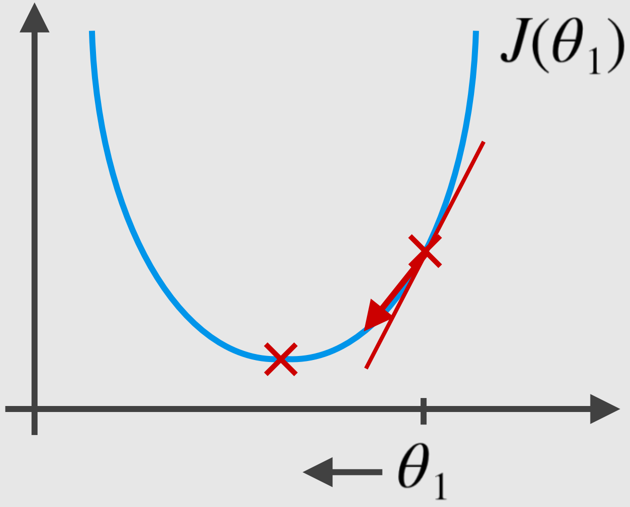


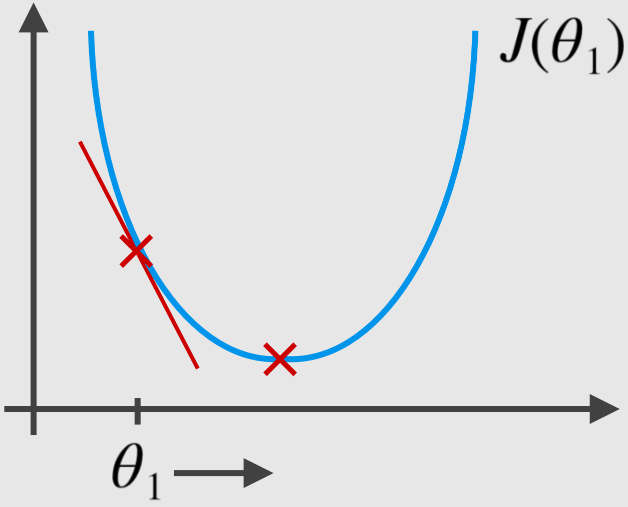
$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$

≤ 0

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

$\theta_1 \in \mathbb{R}$





$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)} \quad \geq 0$$

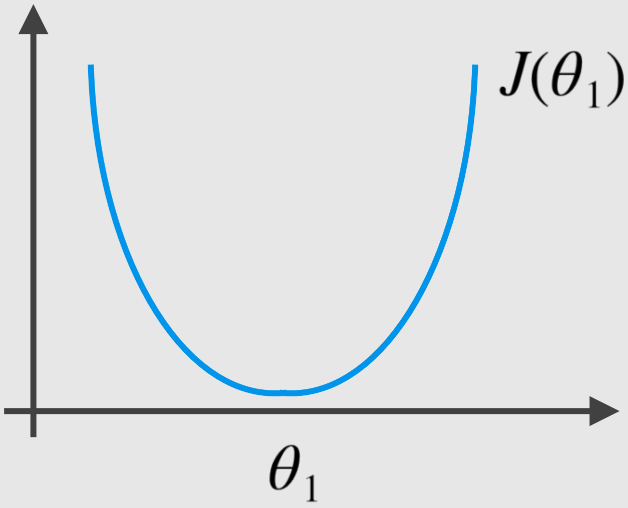
$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$

$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)} \quad \leq 0$$

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

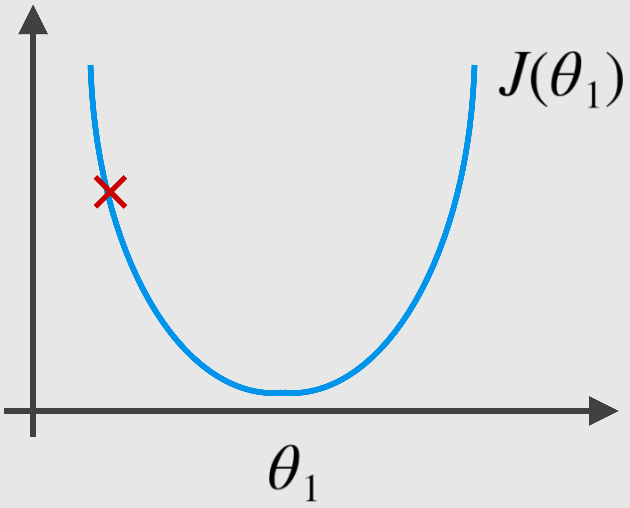
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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

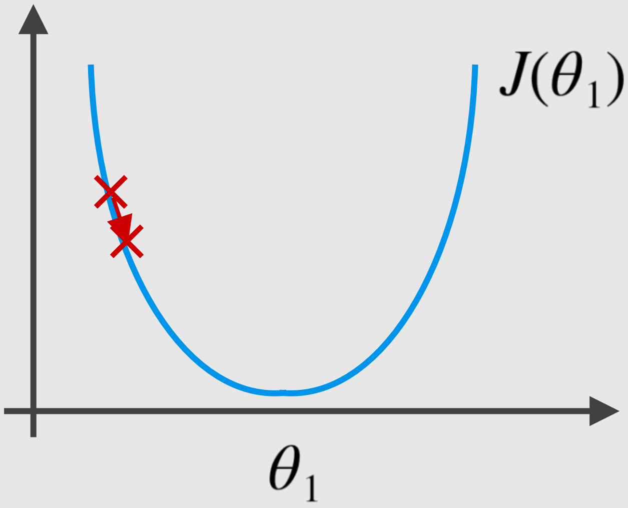


$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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



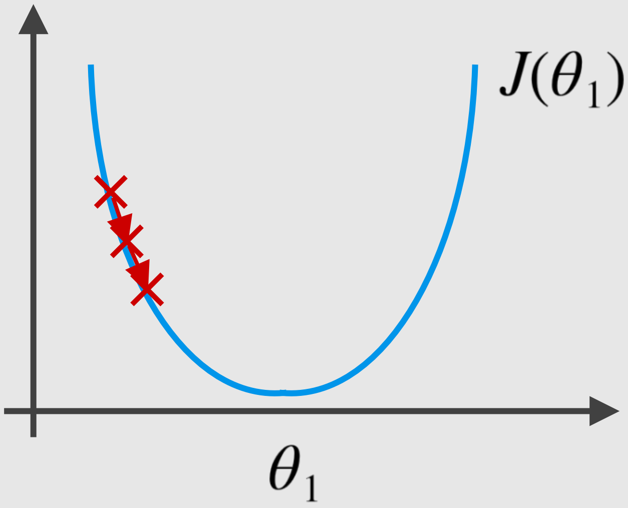
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$



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

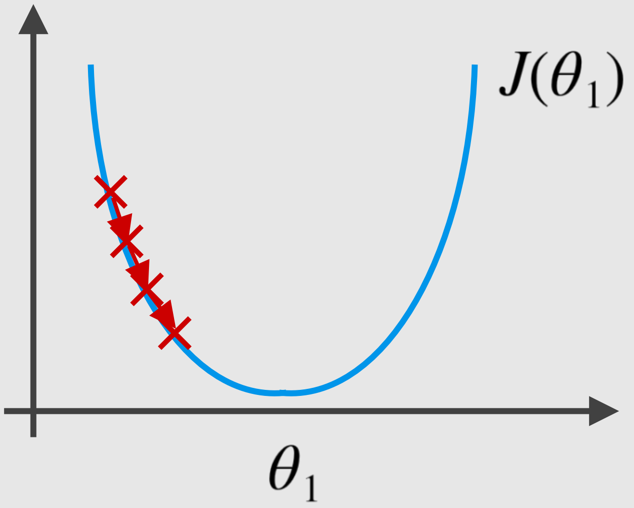
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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



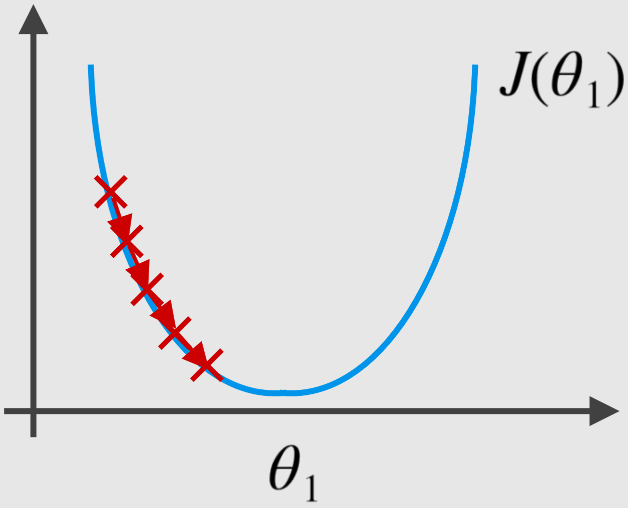
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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



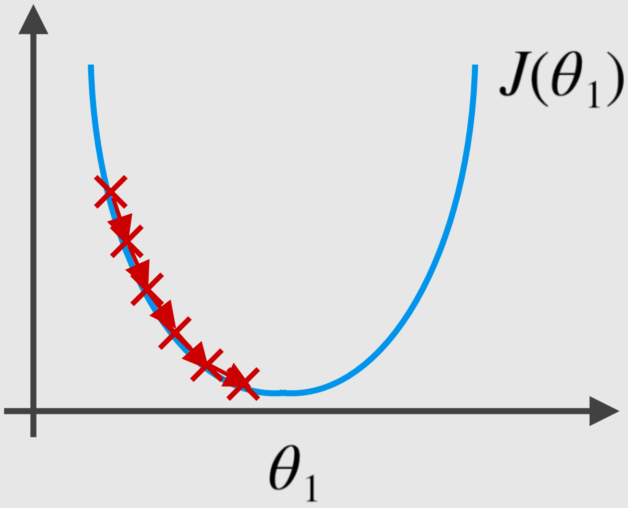
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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



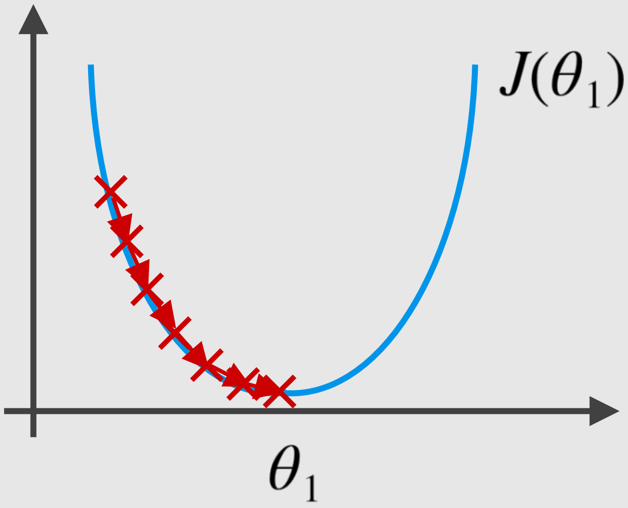
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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



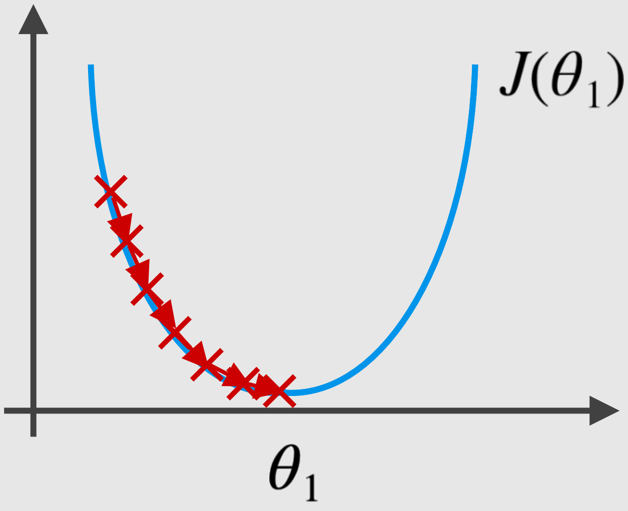
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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

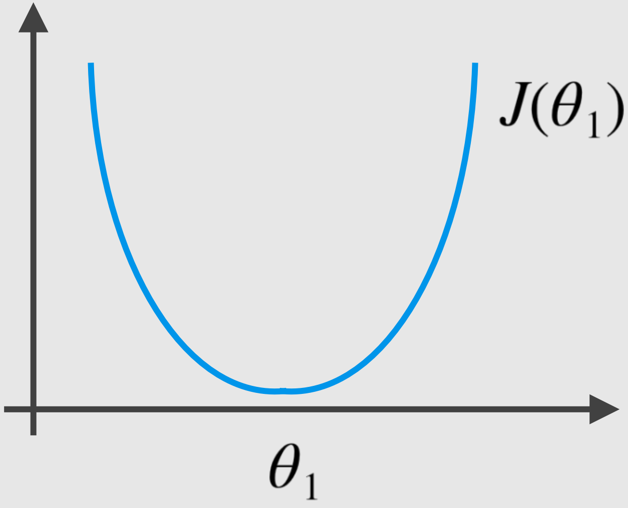


$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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

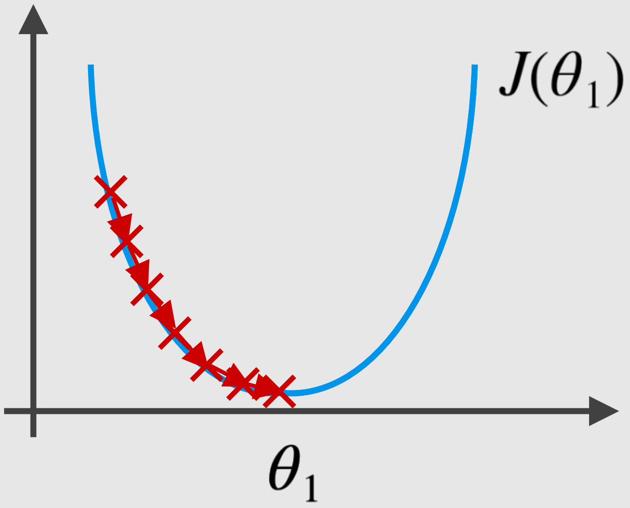


If α is too large, gradient descent can be ...



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

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



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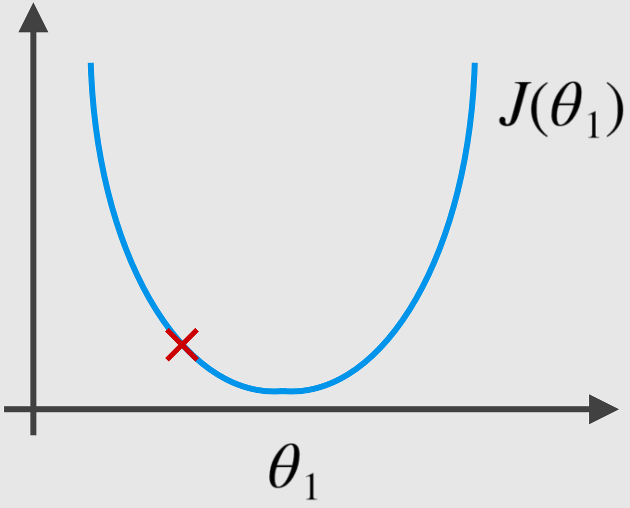

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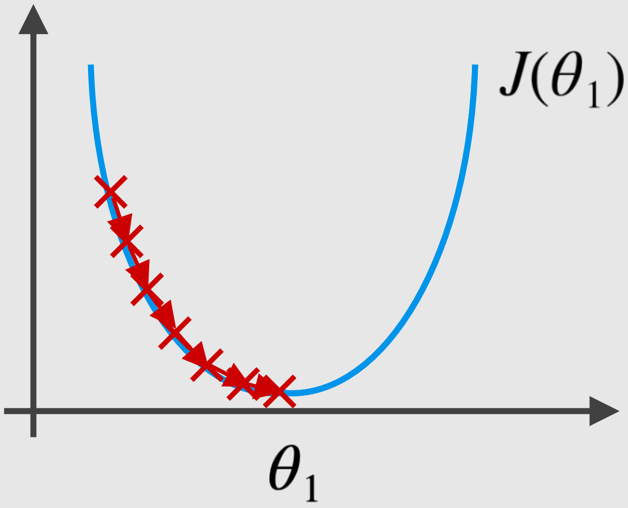

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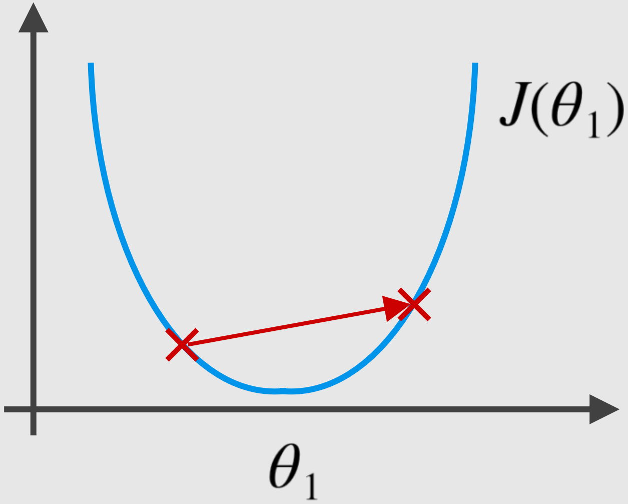

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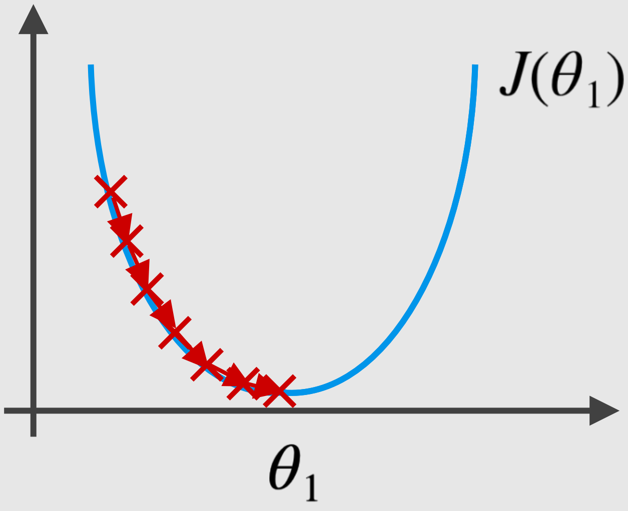

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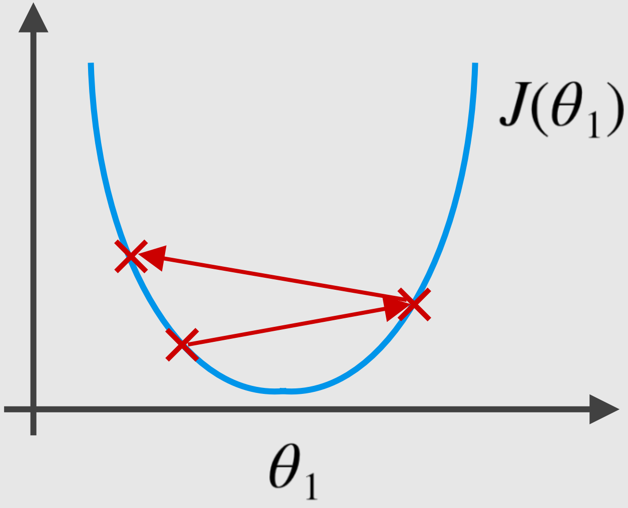

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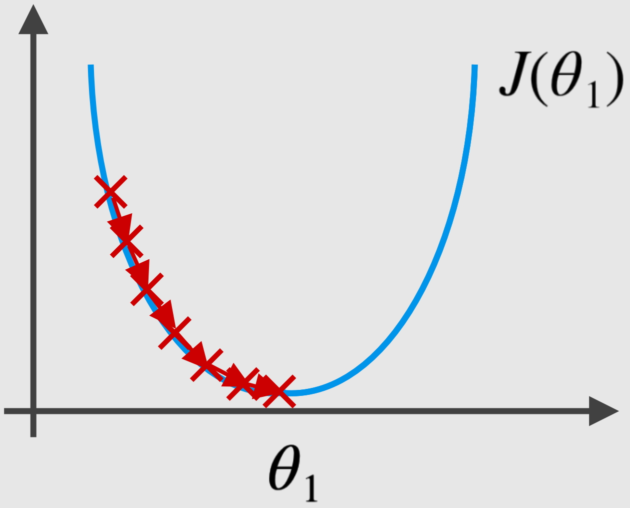

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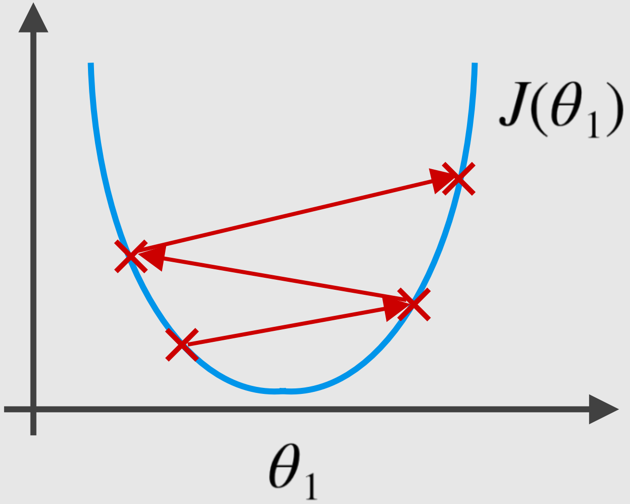

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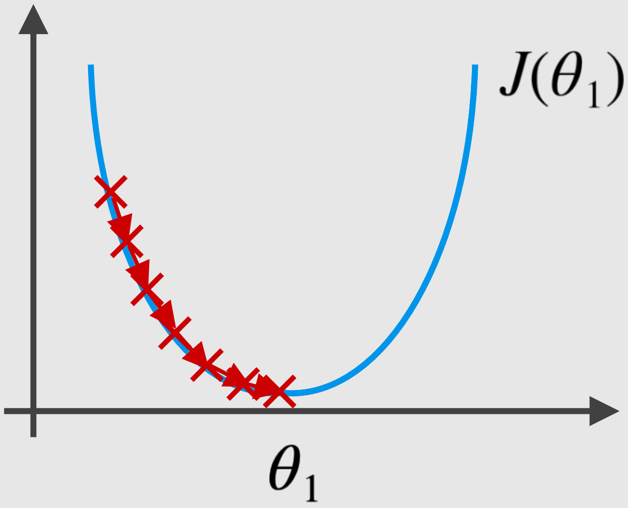

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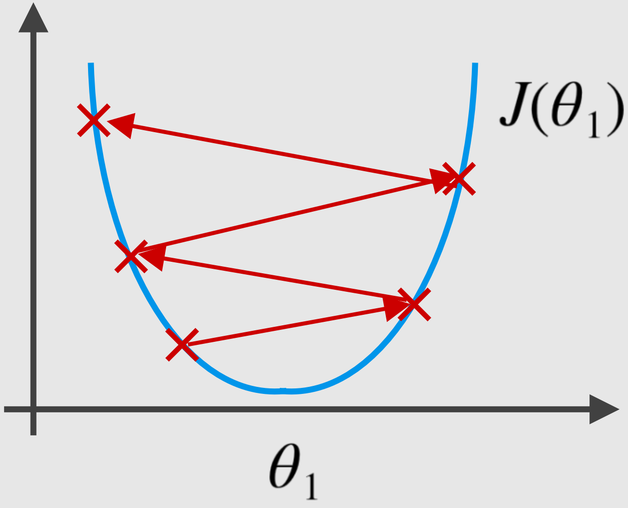
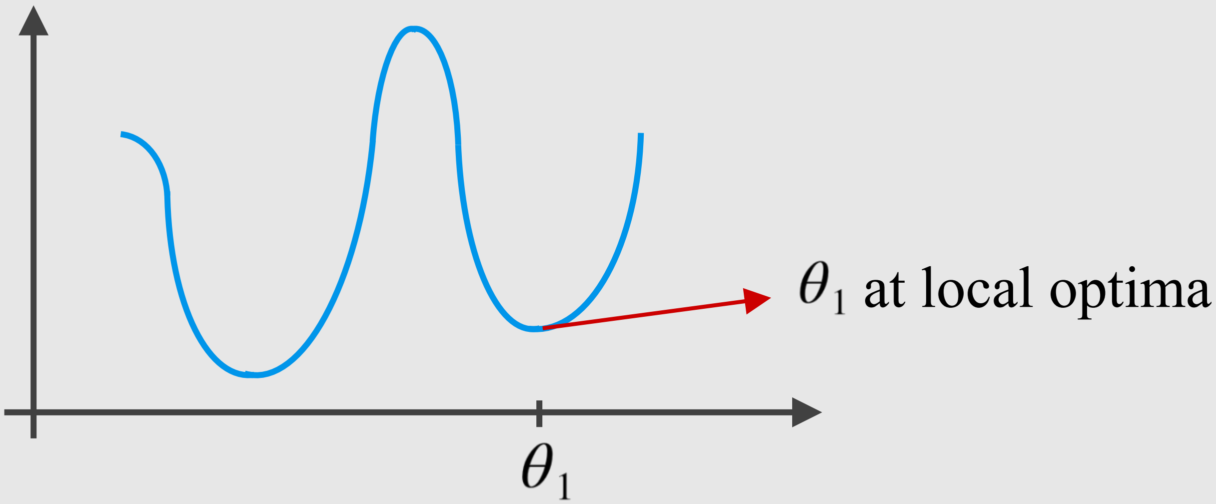


What will one step of gradient descent $\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$ do?



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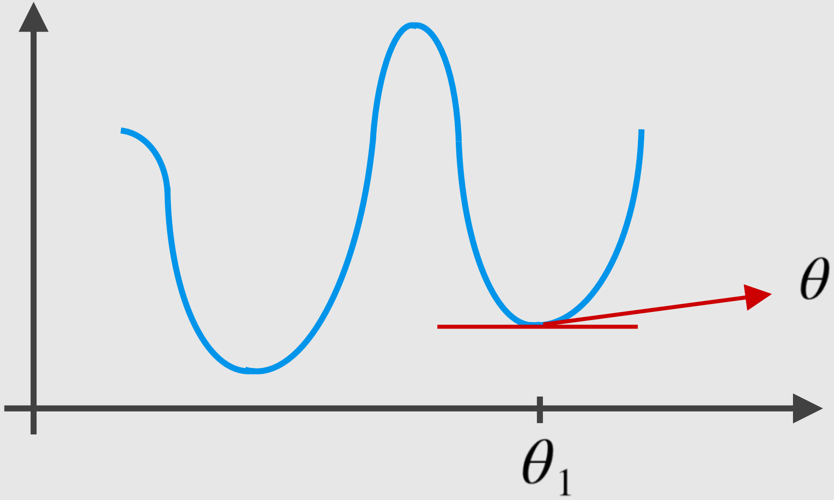
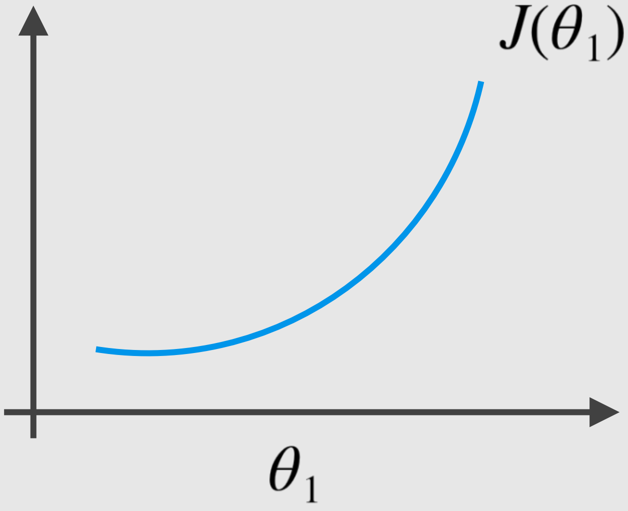
$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$



θ_1 at local optima $= 0$

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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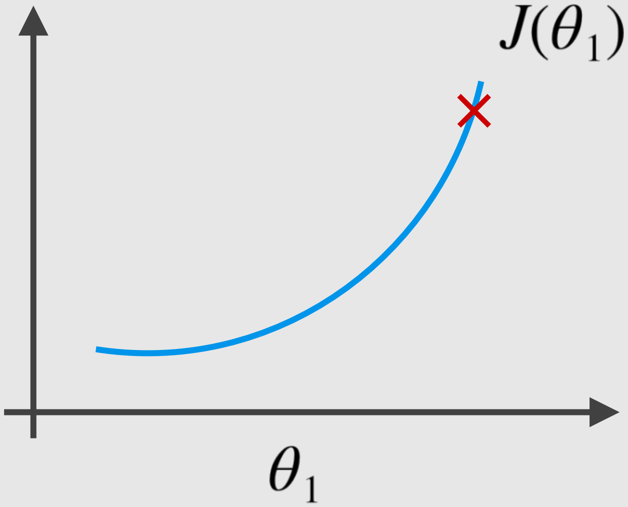

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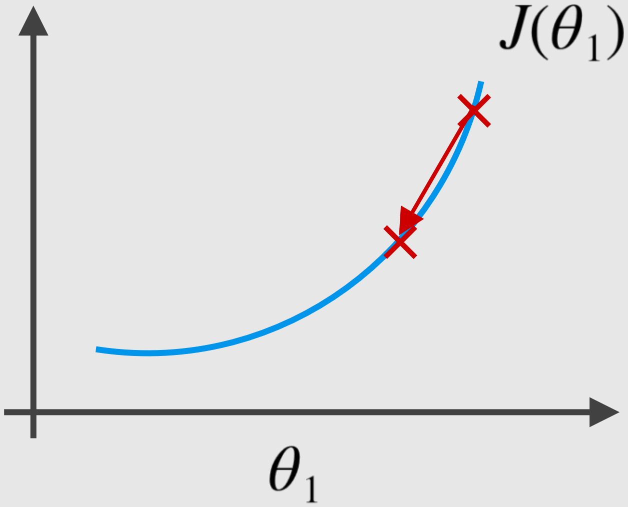

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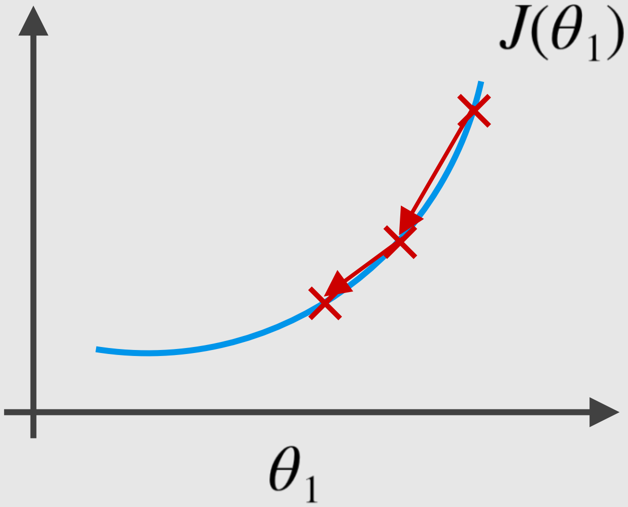

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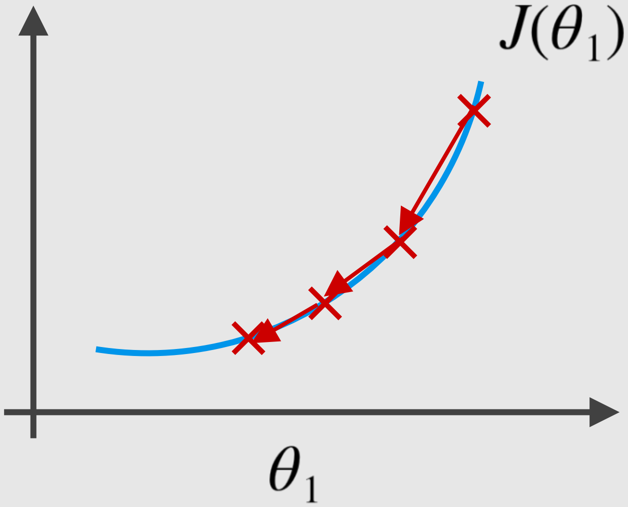

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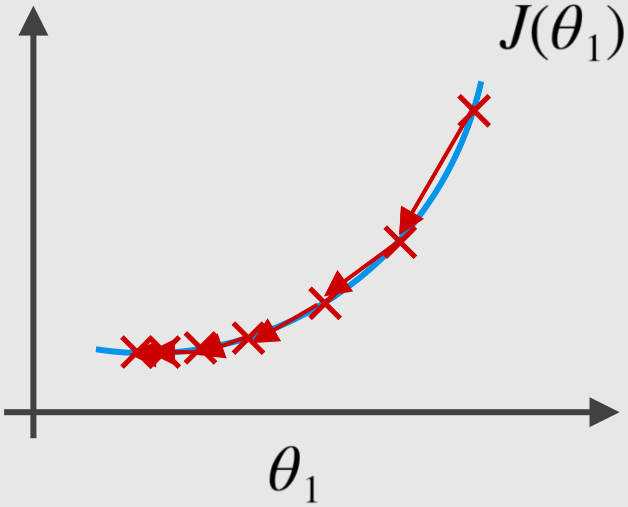

Gradient Descent algorithm

repeat until convergence {

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

(for $j = 0$ and $j = 1$)

}

Linear Regression Model

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

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

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$$\boxed{\underset{\theta_0, \theta_1}{\text{minimize}}\, J(\theta_0, \theta_1)}$$

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

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

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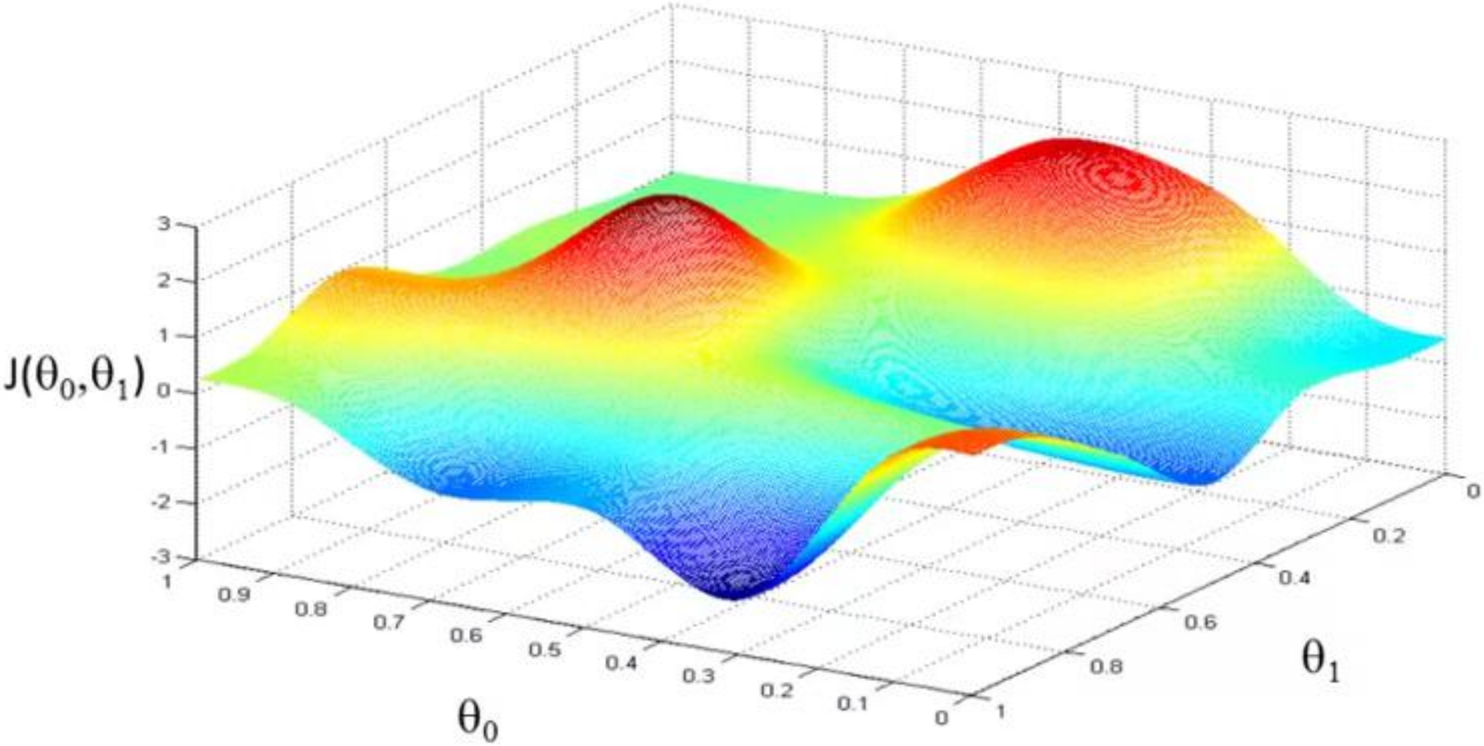
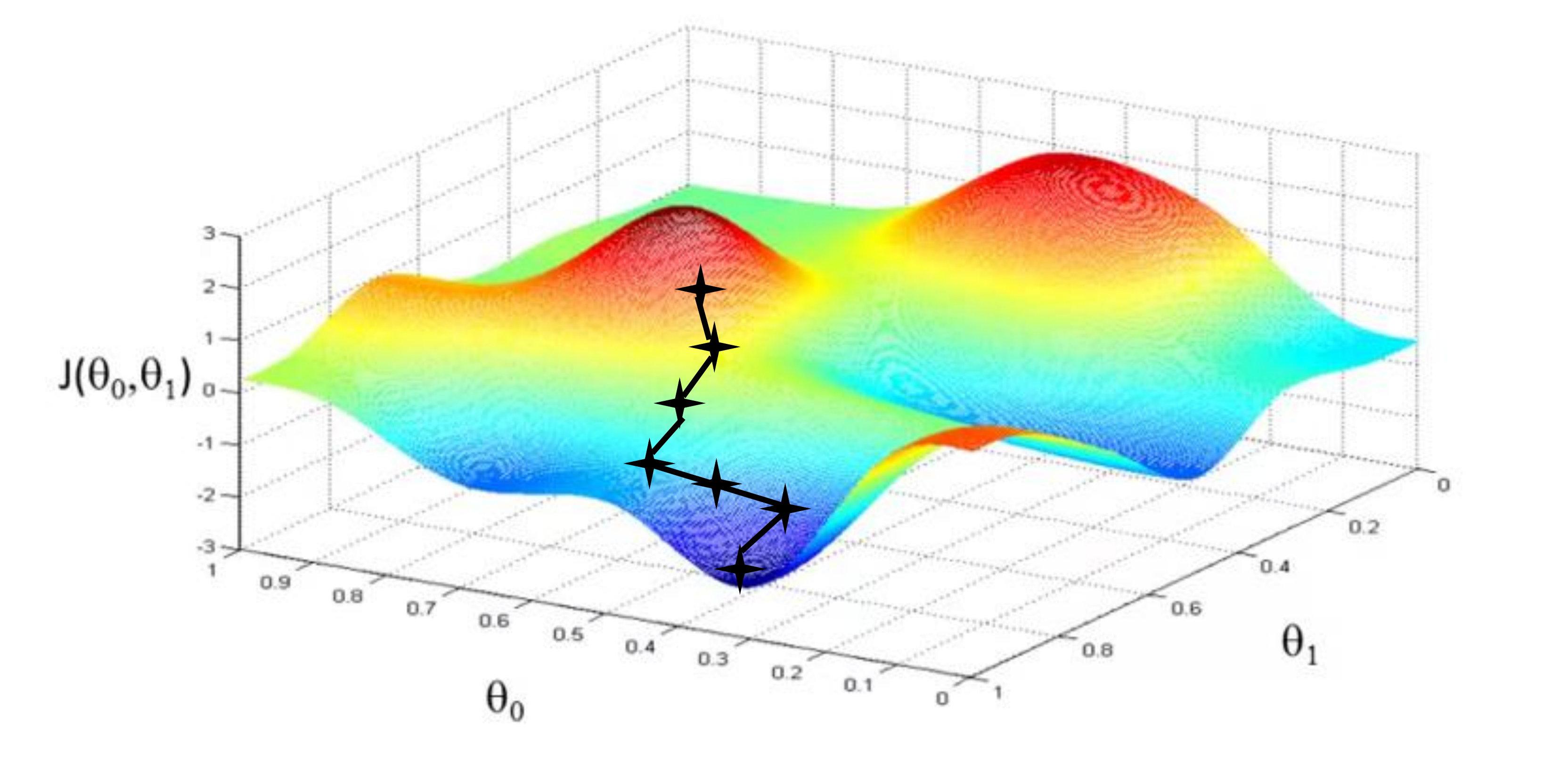
update θ_0 and θ_1 simultaneously

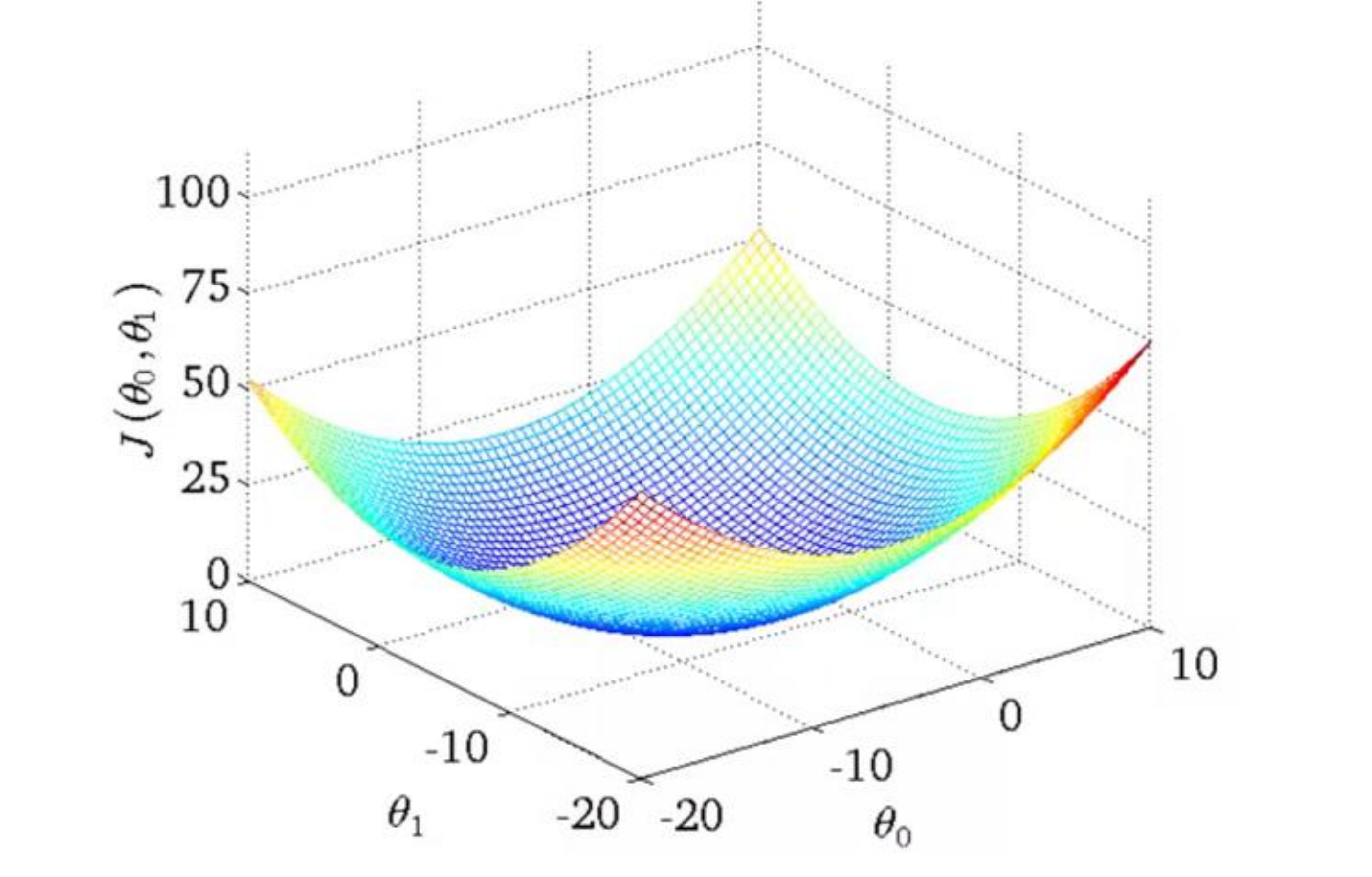
}



3
2
1
0
-1
-2
-3
J(θ0,θ1)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1



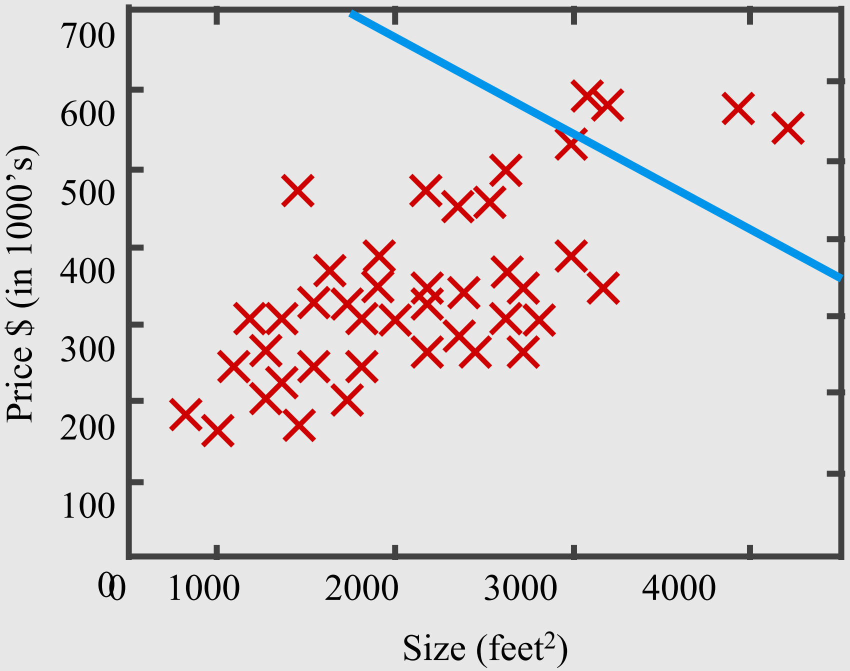
J(θ0,θ1)
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1



$J(\theta_0, \theta_1)$
100
75
50
25
0
10
0
-10
-20
θ_1
-20
-10
0
10
θ_0

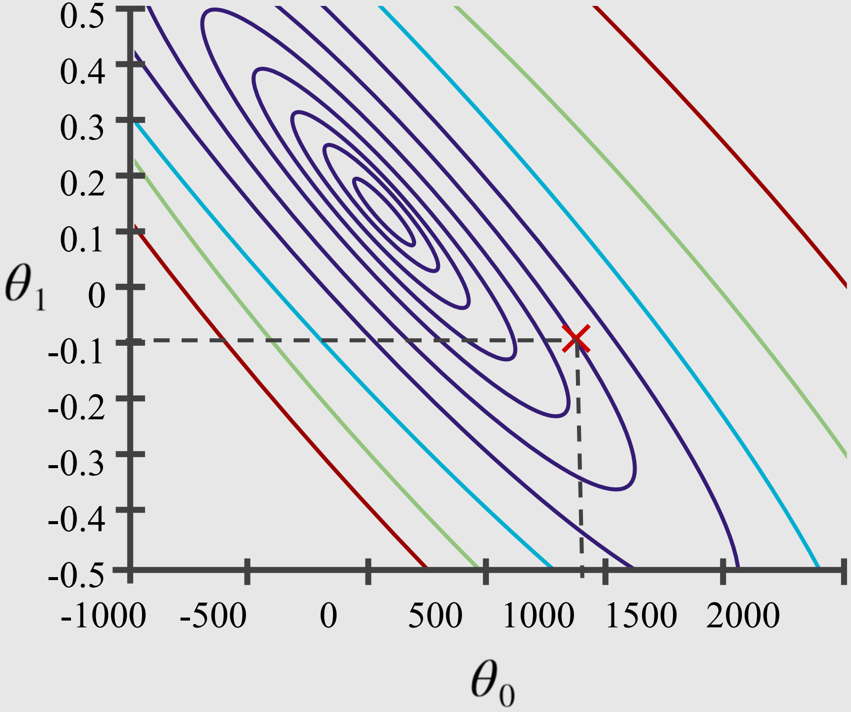
$h_\theta(x)$

(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)



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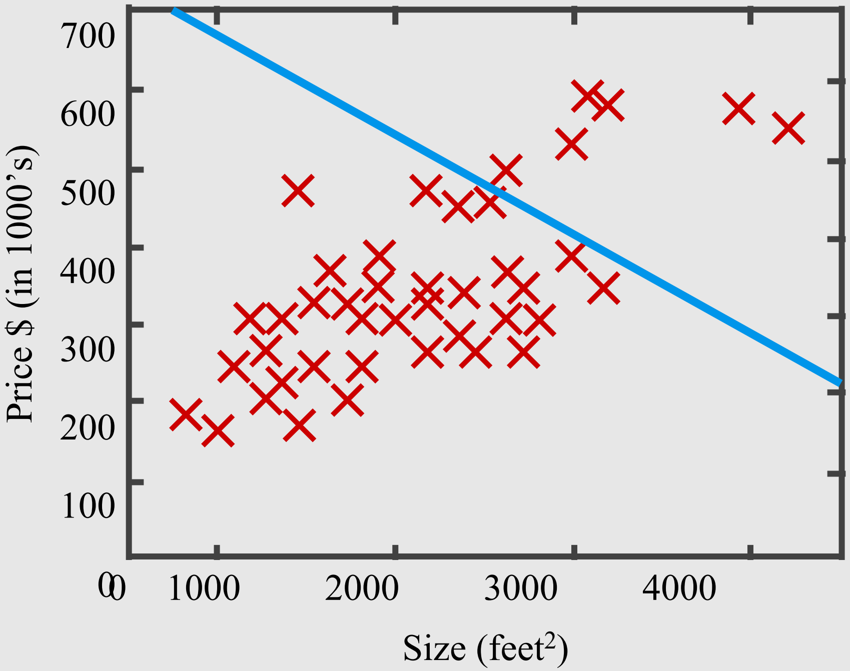

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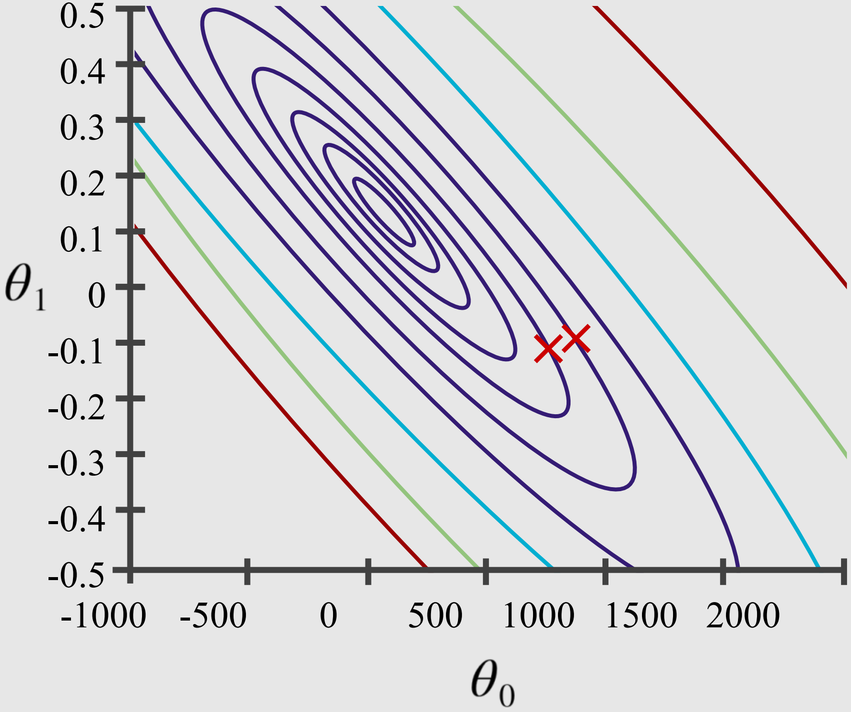

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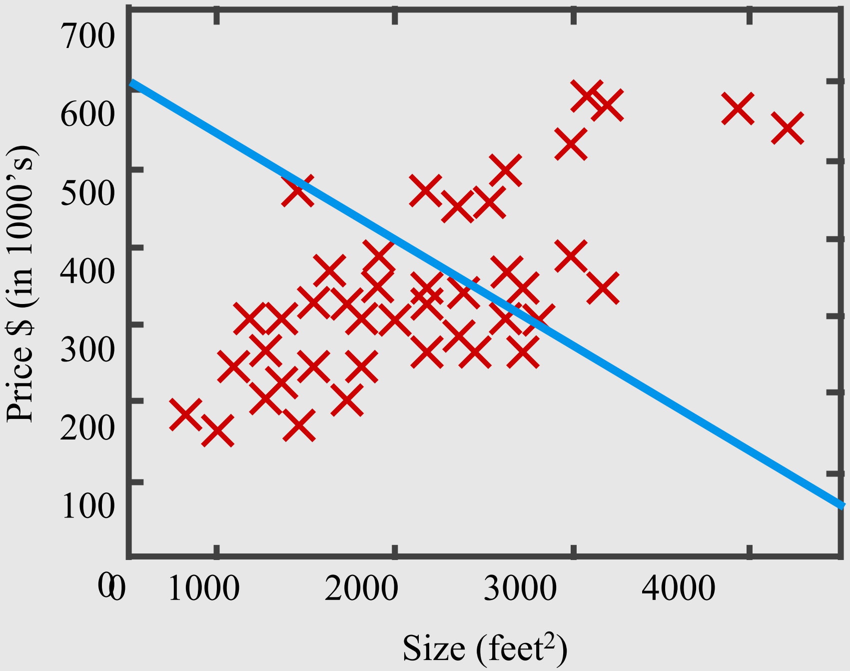

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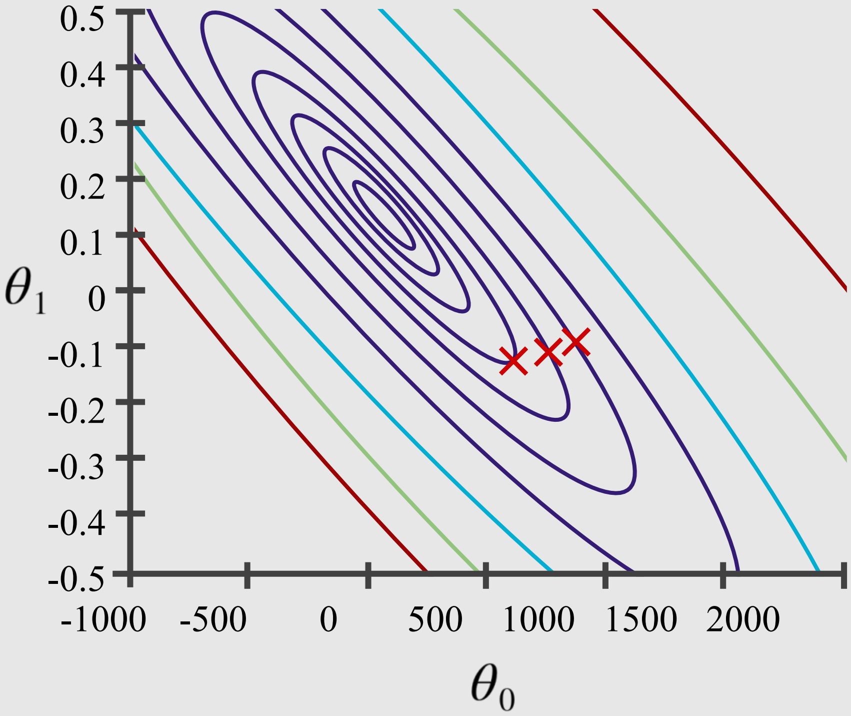

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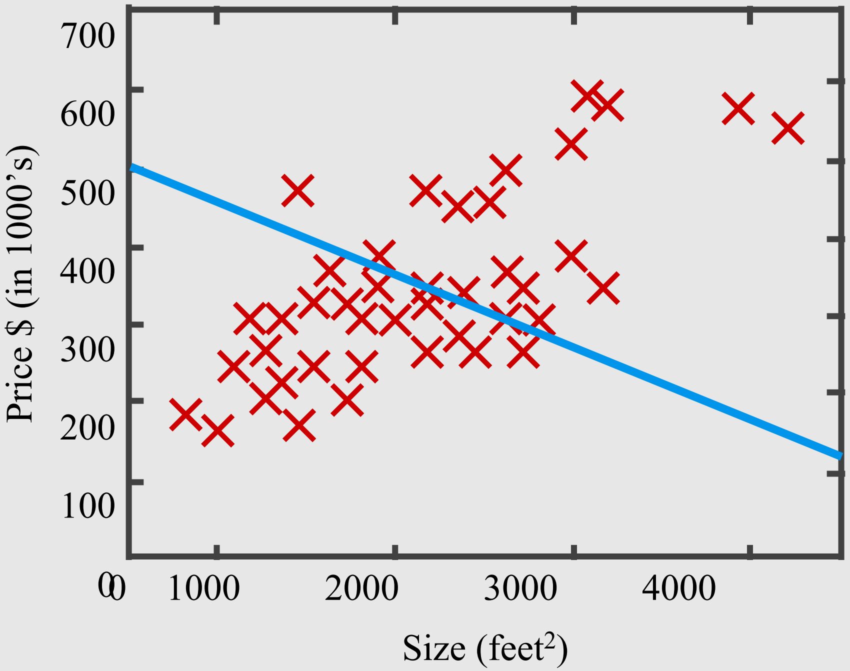

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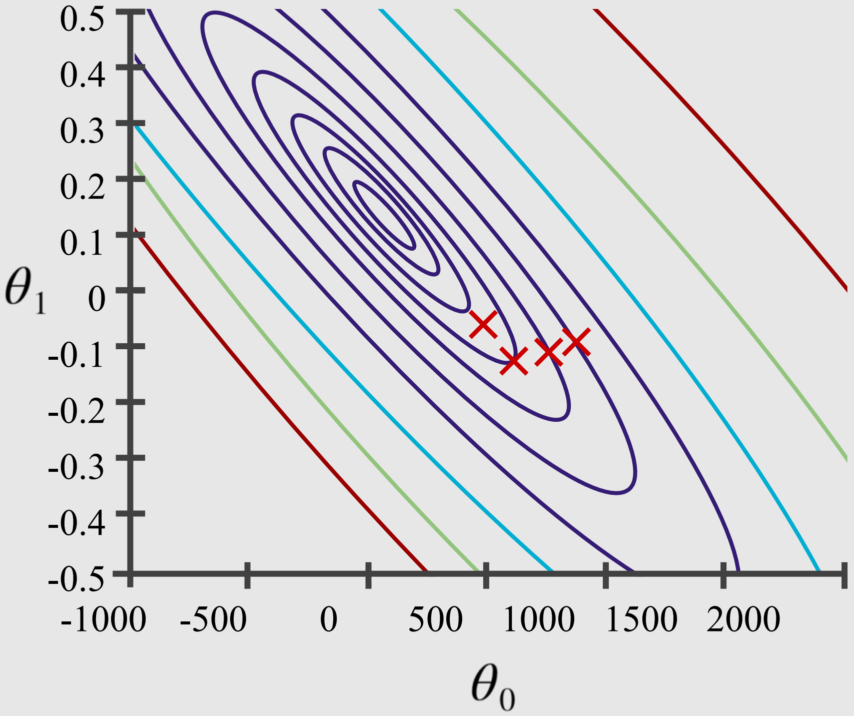

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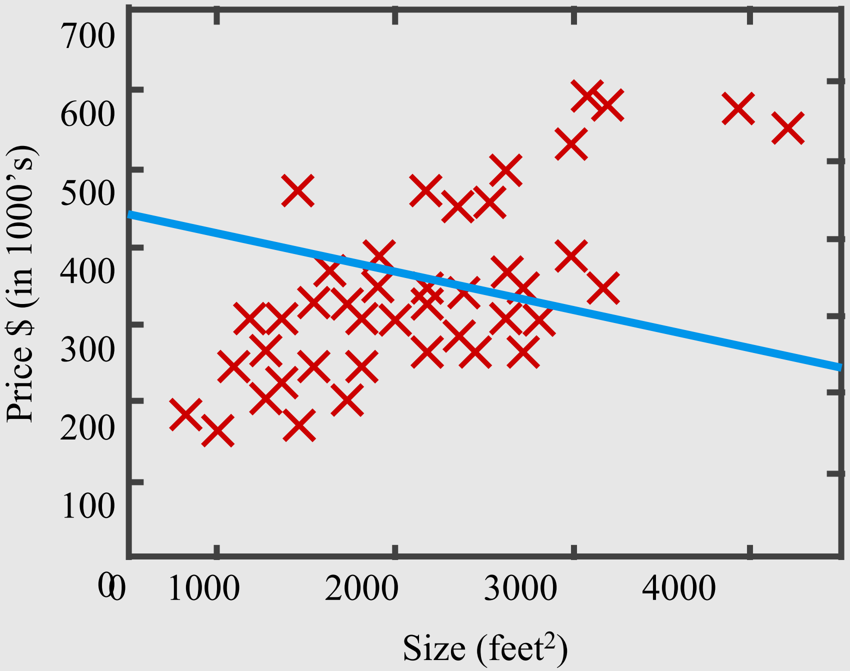

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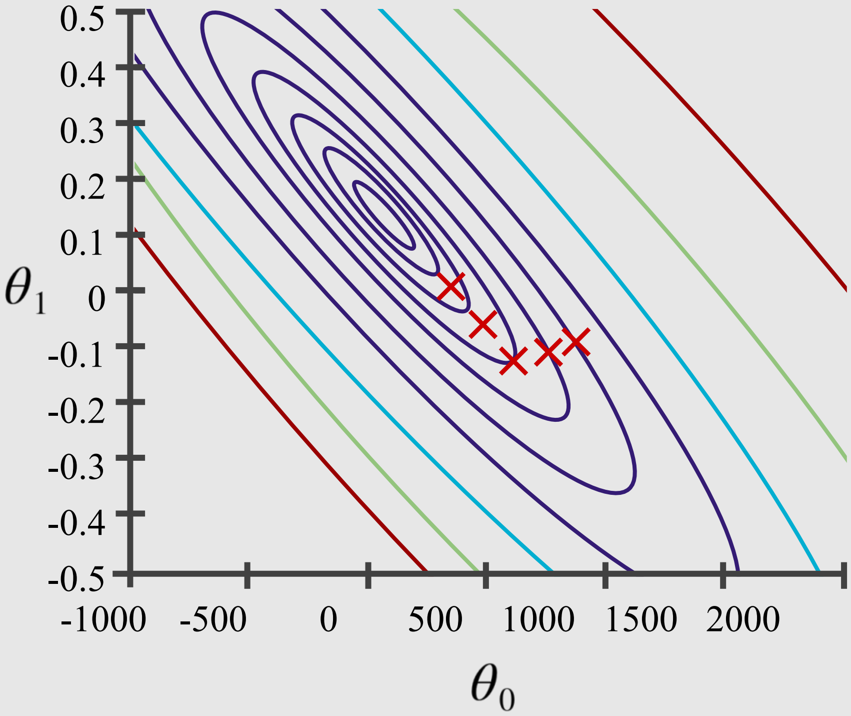

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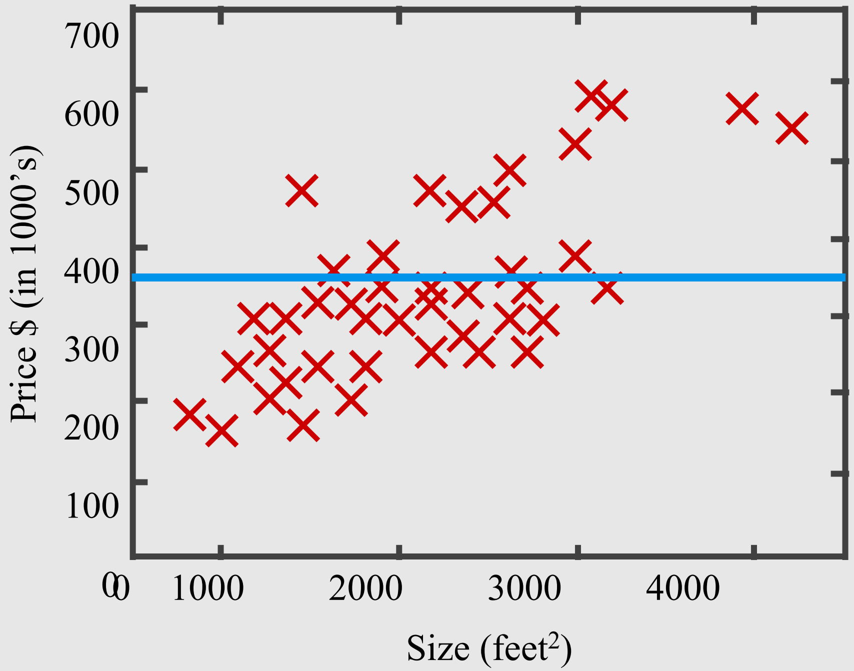

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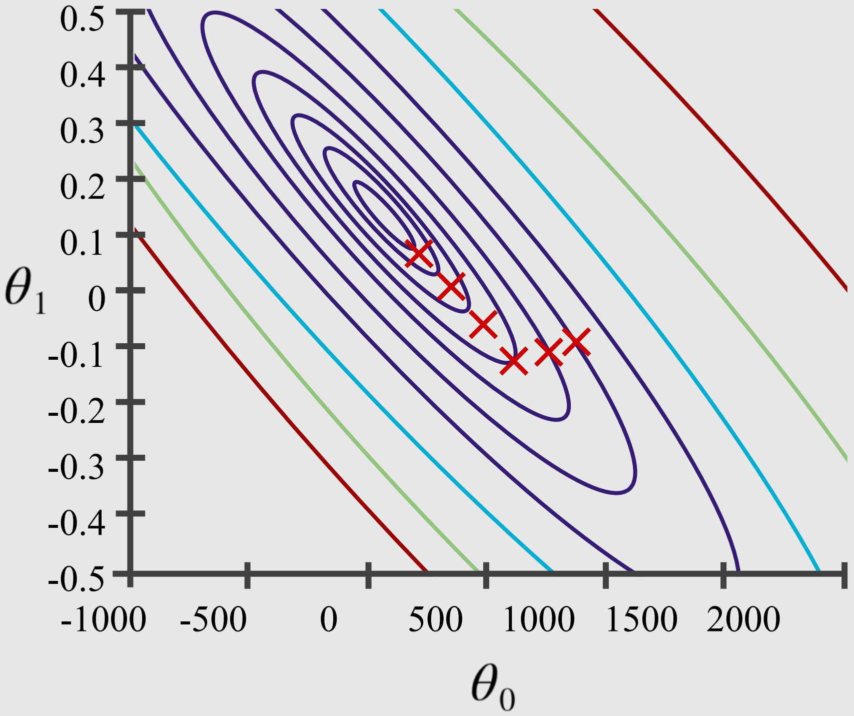

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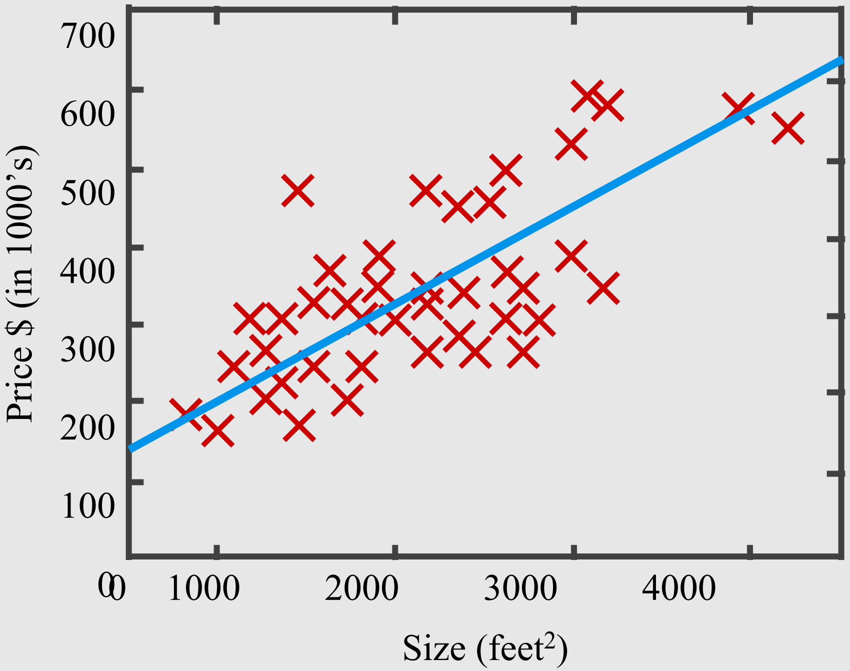

$J(\theta_0,\theta_1)$

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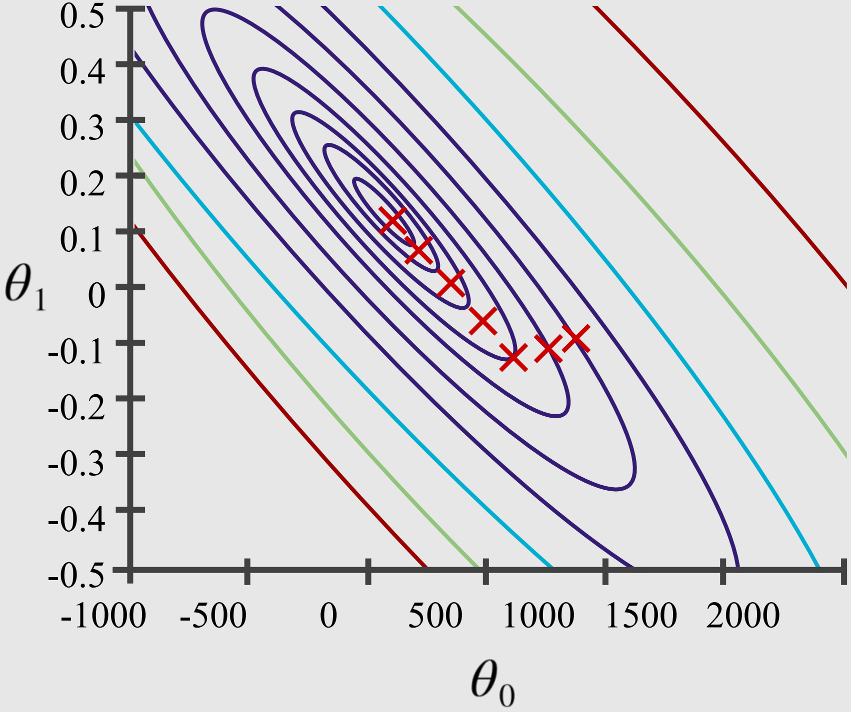
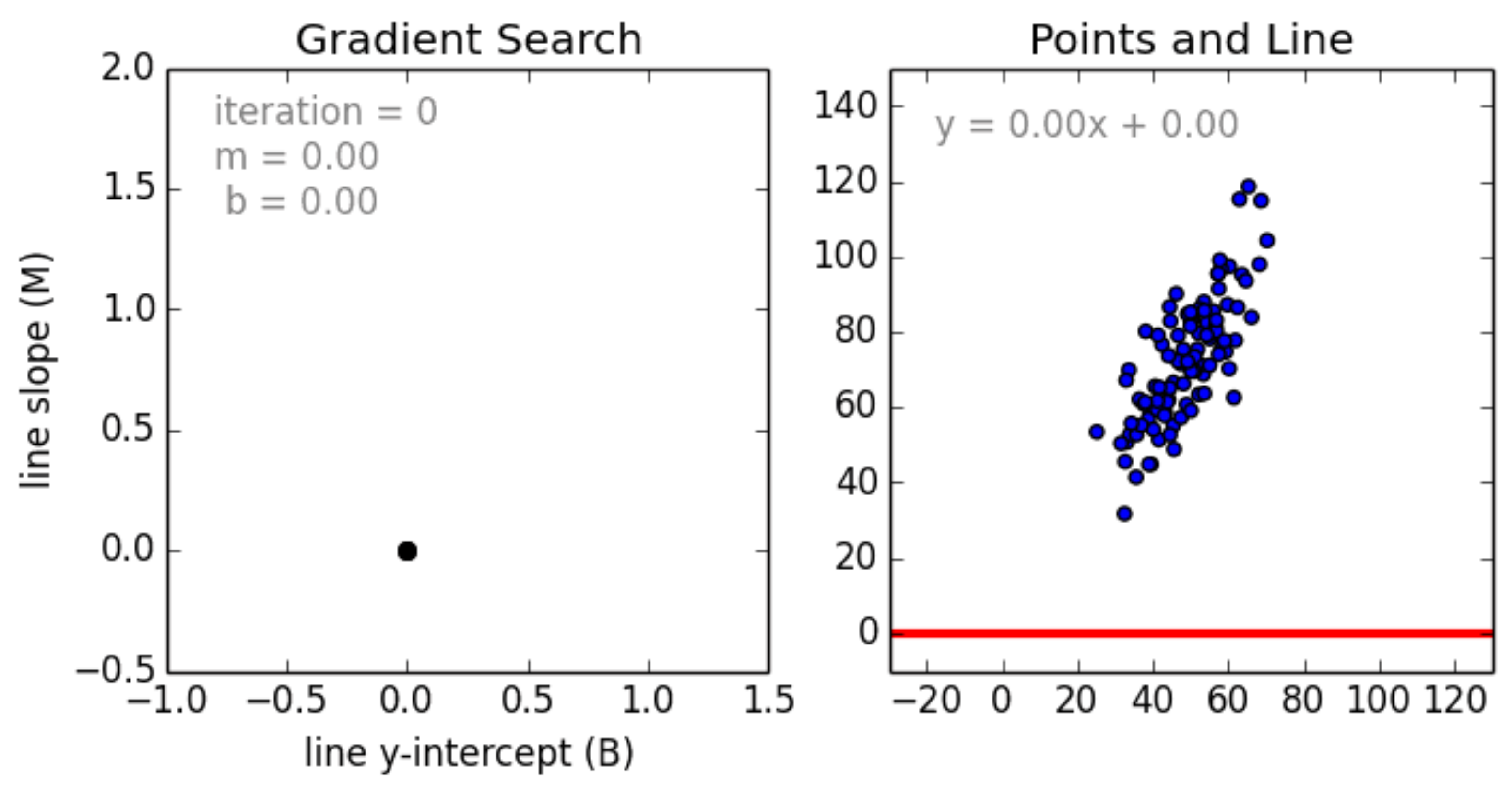


$$h_\theta(x) = \theta_0 + \theta_1 x \quad \Rightarrow \quad y = b + mx$$



Credit: https://github.com/mattnedrich/GradientDescentExample/raw/master/gradient_descent_example.gif

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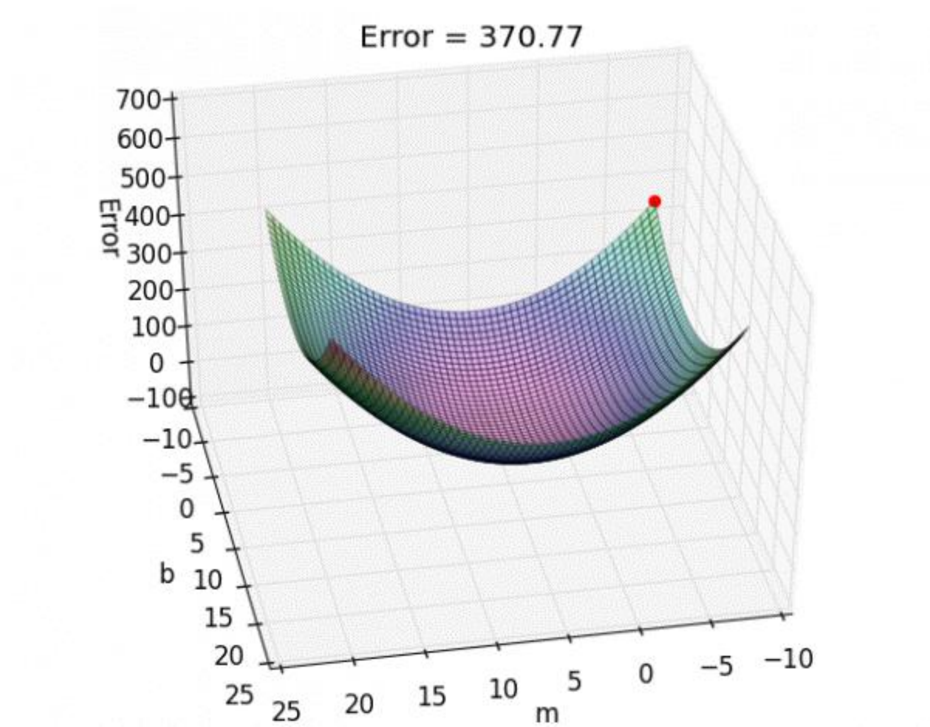

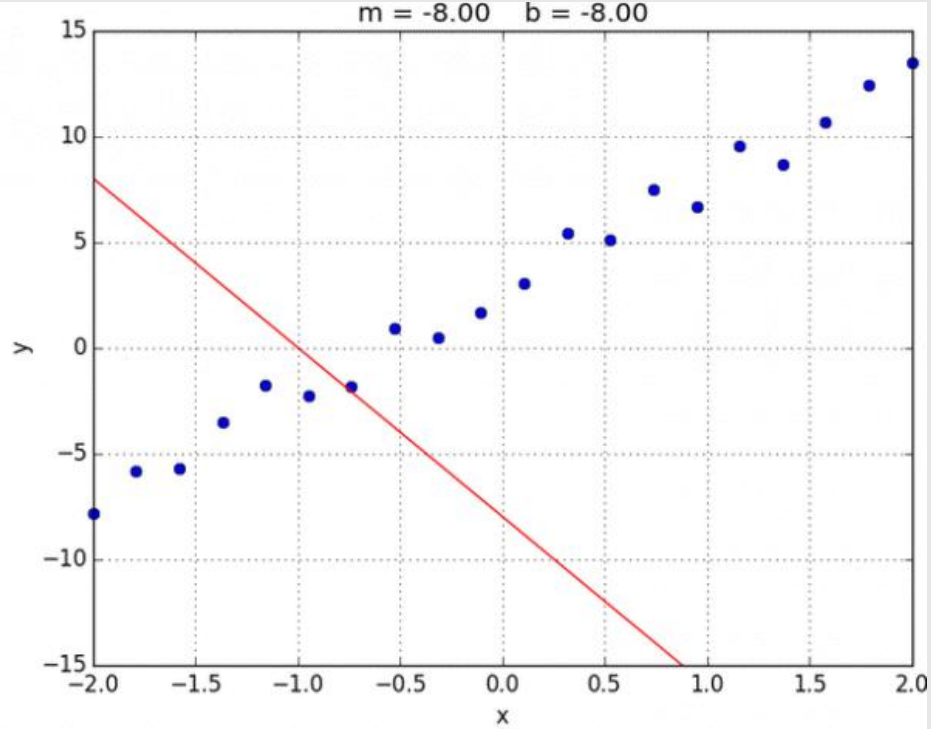

Credit: https://alykhantejani.github.io/a-brief-introduction-to-gradient-descent/

“Batch” Gradient Descent

“Batch”: Each step of gradient descent uses **all the training examples**.

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- Stochastic Gradient Descent
- Mini-batch Gradient Descent

"Batch" Gradient Descent

repeat until convergence {

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

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

update θ_0 and θ_1 simultaneously

}

Stochastic Gradient Descent

Each step of gradient descent uses **one training example**.

repeat until convergence {

for $i \coloneqq 1, \ldots, m$ {

$$\theta_0 := \theta_0 - \alpha(h_\theta(x^{(i)}) - y^{(i)})$$

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

}

}

Mini-batch Gradient Descent

Each step of gradient descent uses ***b* training examples**.

Say $b = 10$, $m = 1000$.
repeat until convergence {

for $i \coloneqq 1, 11, 21\ldots, 991$ {

$$\theta_0 := \theta_0 - \alpha \frac{1}{10} \sum_{i=k}^{i+9} (h_\theta(x^{(k)}) - y^{(k)})$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{10} \sum_{i=k}^{i+9} (h_\theta(x^{(k)}) - y^{(k)})\, x^{(k)}$$

} }

Linear Regression with multiple variables

Multiple ~~Variables~~ Features

Size in feet^2 (x)	**Price ($) in 1000's ($y$)**
2104	460
1416	232
1534	315
852	178
...	...

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

Multiple ~~Variables~~ Features

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

Notation:

n = number of features

$x^{(i)}$ = input (features) of i^{th} training example

$x_j^{(i)}$ = value of features j in i^{th} training example

Hypothesis

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

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

Hypothesis

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

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

$$h_\theta(x) = 80 + 0.1 x_1 + 10 x_2 + 3 x_3 - 2 x_4$$

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

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For convenience of notation, define $x_0 = 1$.

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

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For convenience of notation, define $x_0 = 1$.

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

$$\begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$h_\theta(x) = \theta^T x$$

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

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$$h_\theta(x) = \theta^T x$$

Multivariate linear regression.

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

Parameters: $\theta_0, \theta_1, \ldots, \theta_n$

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

Gradient Descent:

repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1, \ldots, \theta_n)$$

} (simultaneously update for every $j = 0, 1, \ldots, n$)

Gradient Descent

Previously ($n = 1$):

repeat {

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

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

(simultaneously update θ_0, θ_1)

}

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New Algorithm ($n \geq 1$):

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

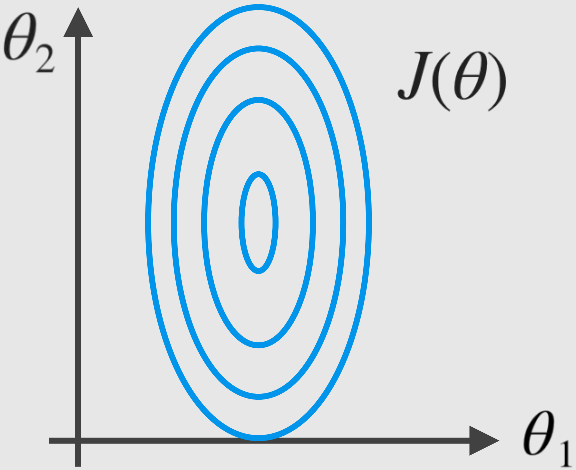
...

Feature Scaling

Feature Scaling

Idea: Make sure features are on similar scale.

E.g. x_1= size (0–2000 feet^2)
x_2= number of bedrooms (1–5)



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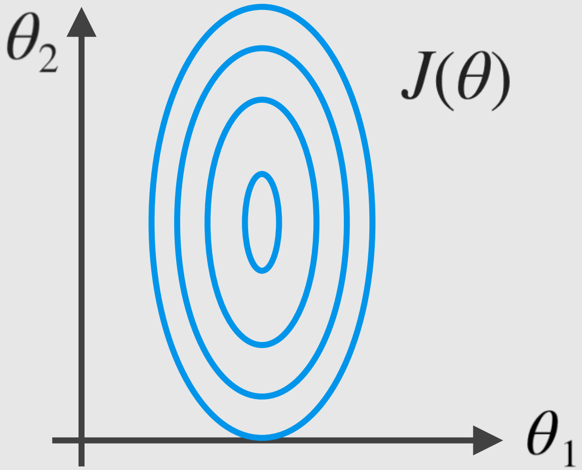

$$x_1 = \frac{\text{size (feet}^2)}{2000}$$

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

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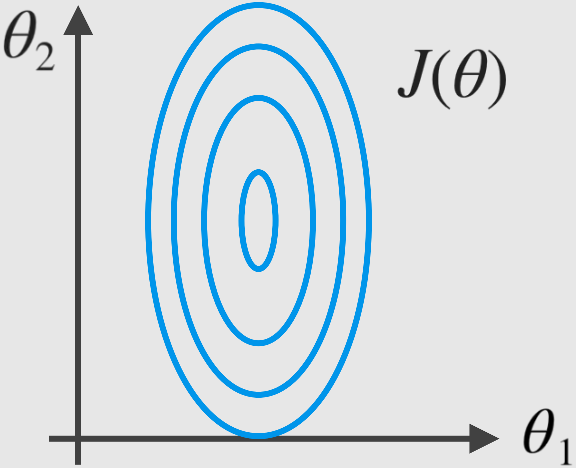

$$x_1 = \frac{\text{size (feet}^2)}{2000}$$

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

Feature Scaling

Get every feature into approximately a $-1 \leq x_i \leq 1$ range.

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. $x_1 = \dfrac{\text{size} - 1000}{2000}$ ➡ $-0.5 \le x_1 \le 0.5$

$x_2 = \dfrac{\#\text{bedrooms} - 2.5}{5}$ ➡ $-0.5 \le x_2 \le 0.5$

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$x_2 = \dfrac{\#\text{bedrooms} - 2.5}{5}$ ➡ $-0.5 \le x_2 \le 0.5$

$$x_1 = \frac{x_1 - \mu_1}{s_1} \qquad x_2 = \frac{x_2 - \mu_2}{s_2}$$

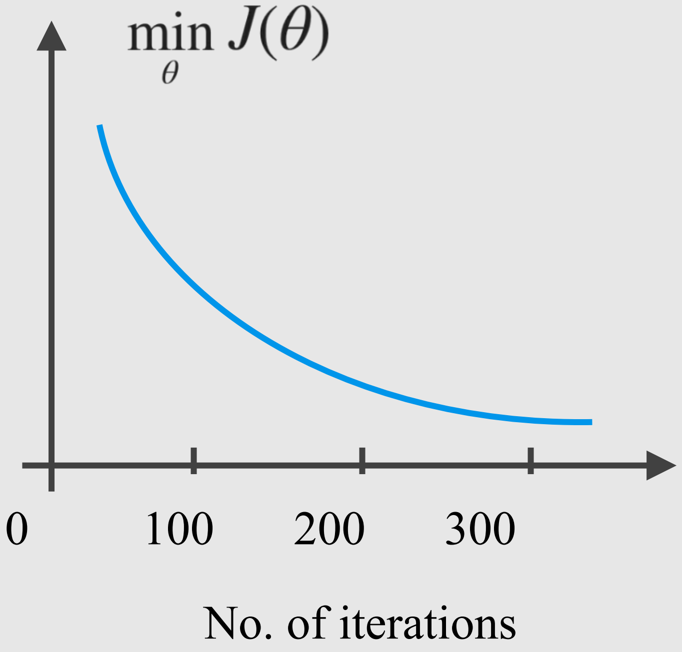
Learning Rate

Gradient Descent

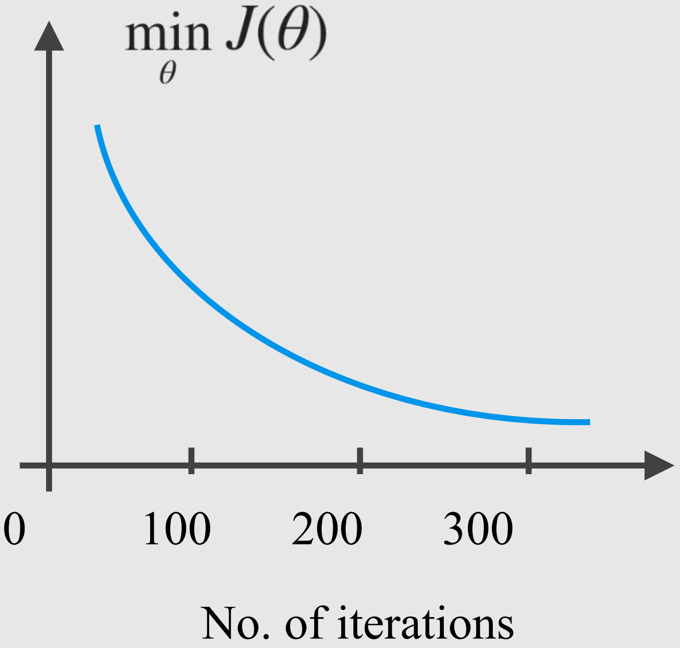
$$\theta_j := \theta_{\mathrm{j}} - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

- "Debugging" : How to make sure gradient descent is working correctly.
- How to choose learning rate α.

Making sure gradient descent is working correctly.



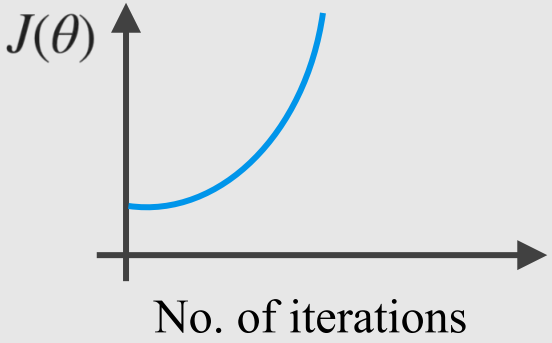
Making sure gradient descent is working correctly.



Example automatic convergence test:

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

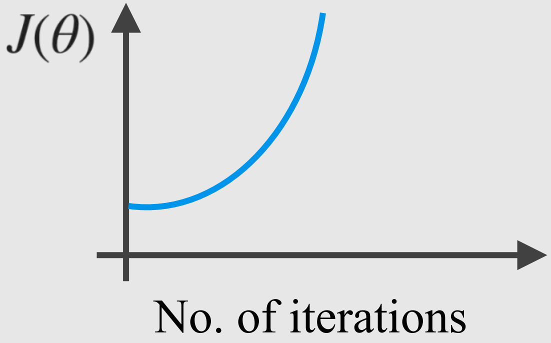
Making sure gradient descent is working correctly.



Gradient descent not working.

Use smaller α.

Making sure gradient descent is working correctly.



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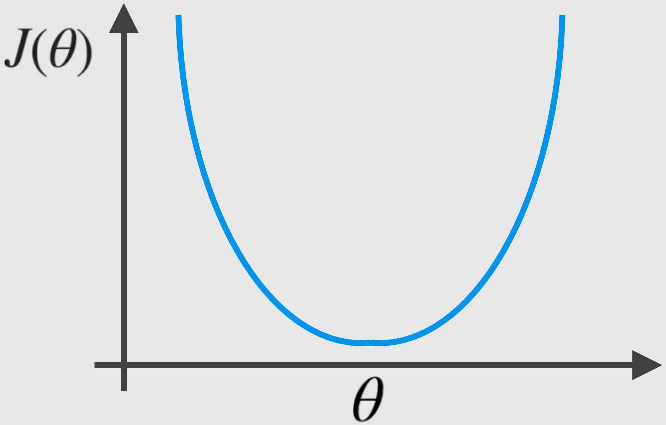

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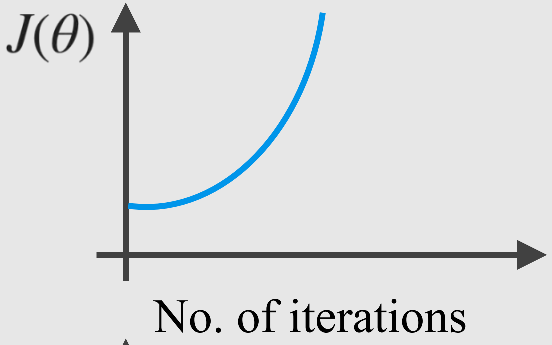

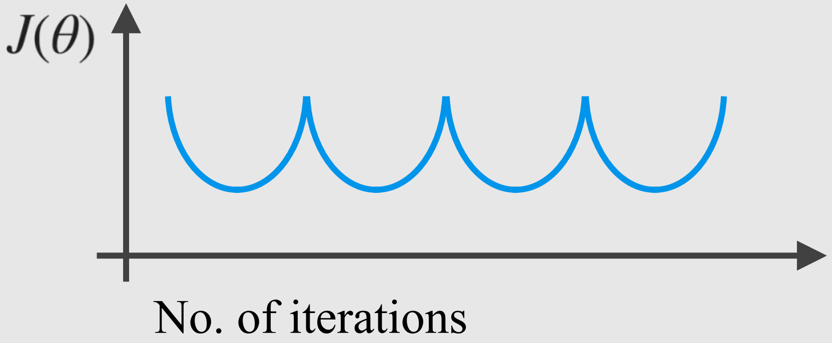

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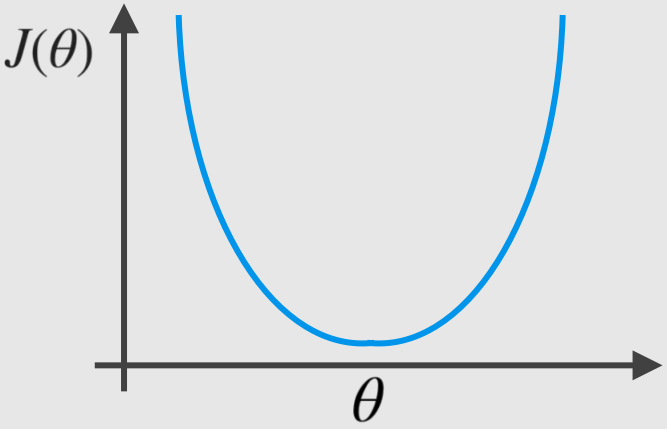

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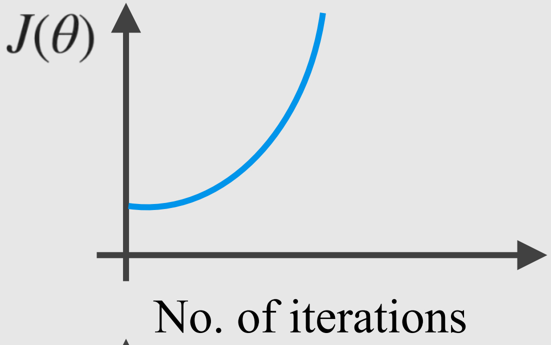

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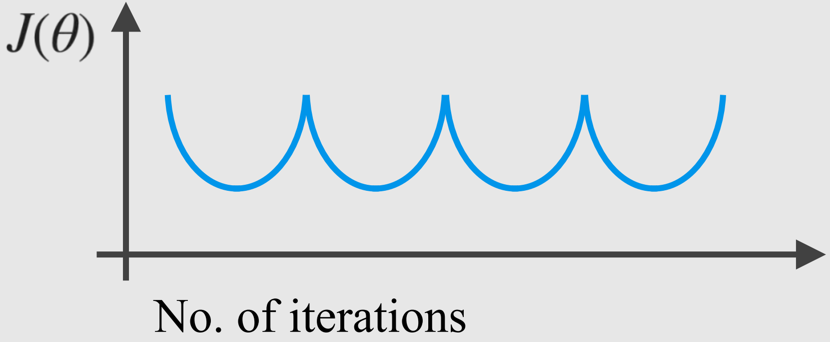

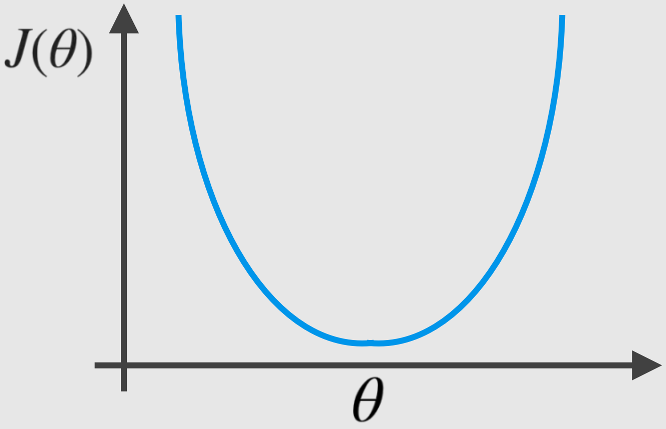

- For sufficiently small α, $J(\theta)$ should decrease on every iteration.
- But if α is too small, gradient descent can be slow to converge.

Summary

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

To choose α, try

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

Features and Polynomial Regression

Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \text{frontage} + \theta_2 \times \text{depth}$$

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Area x = frontage $\times$ depth

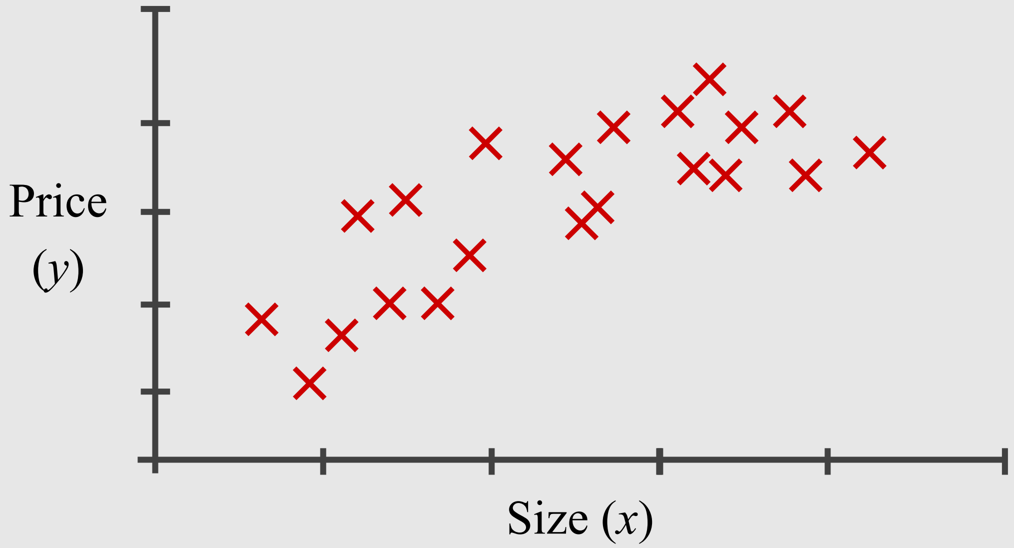
Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \underset{\substack{\Big\downarrow \\ x_1}}{\text{frontage}} + \theta_2 \times \underset{\substack{\Big\downarrow \\ x_2}}{\text{depth}}$$

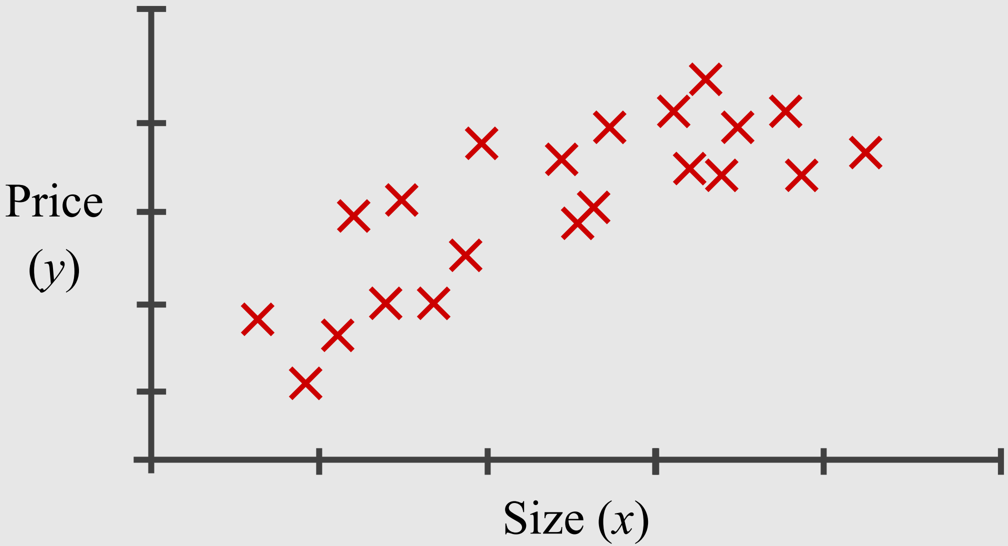
Area x = frontage $\times$ depth

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

Polynomial Regression

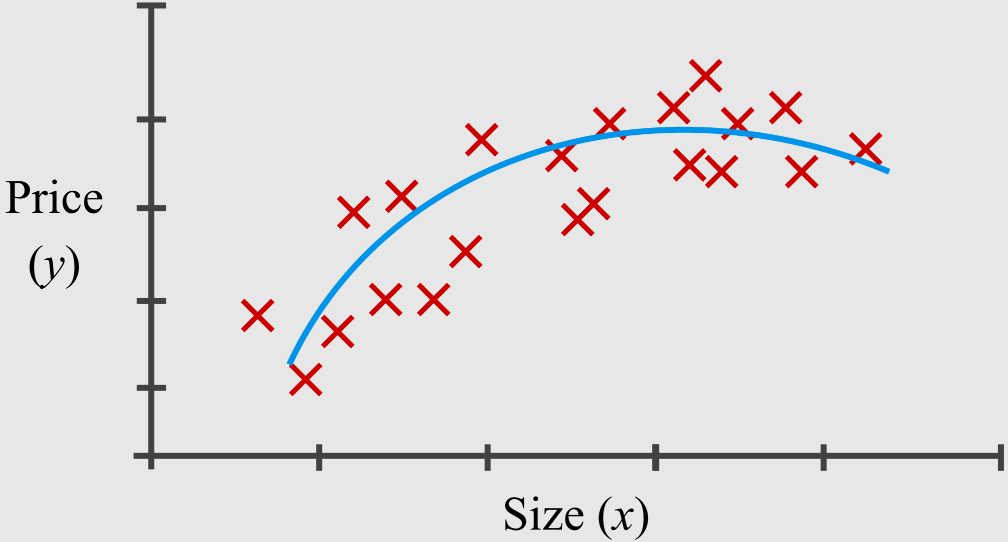


Polynomial Regression



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

Polynomial Regression



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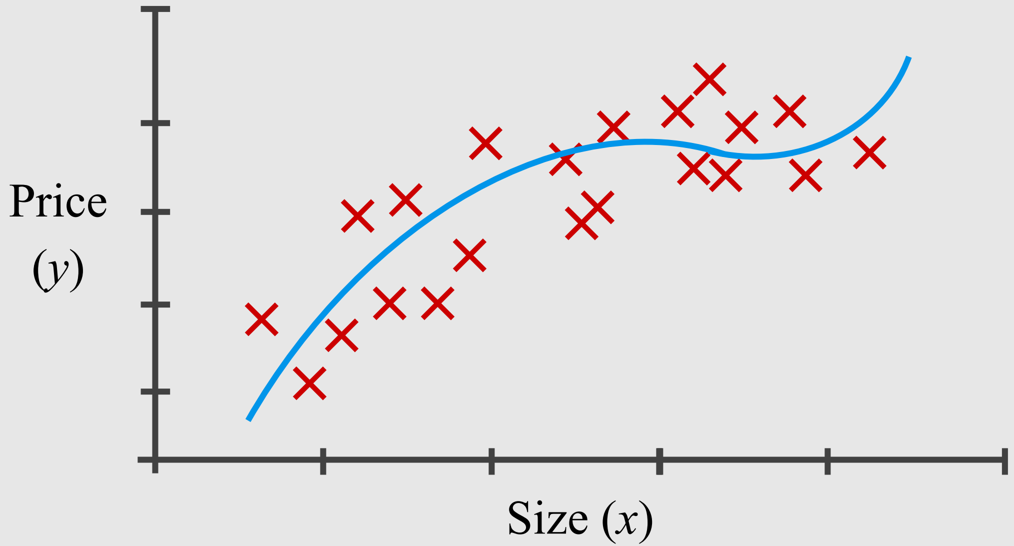

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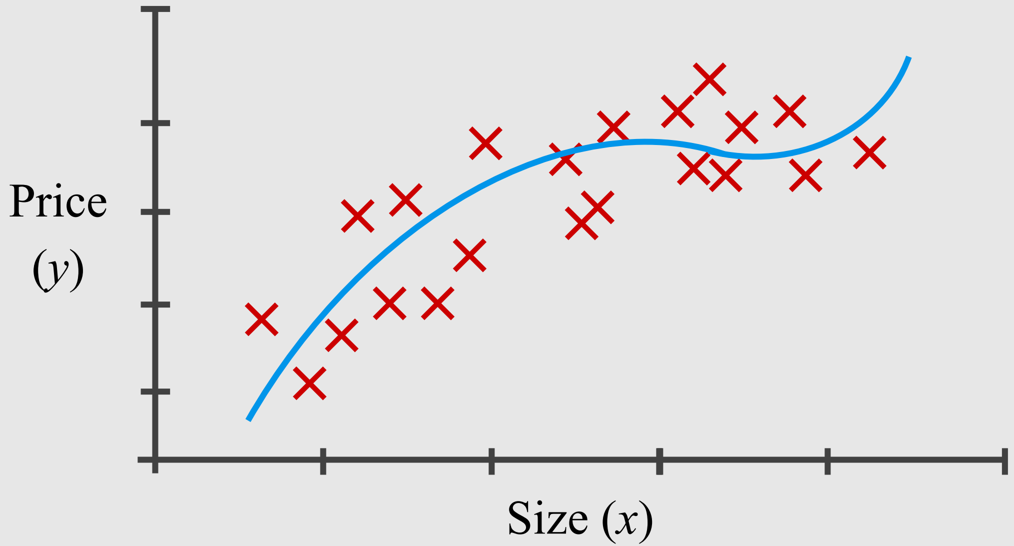
Polynomial Regression



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

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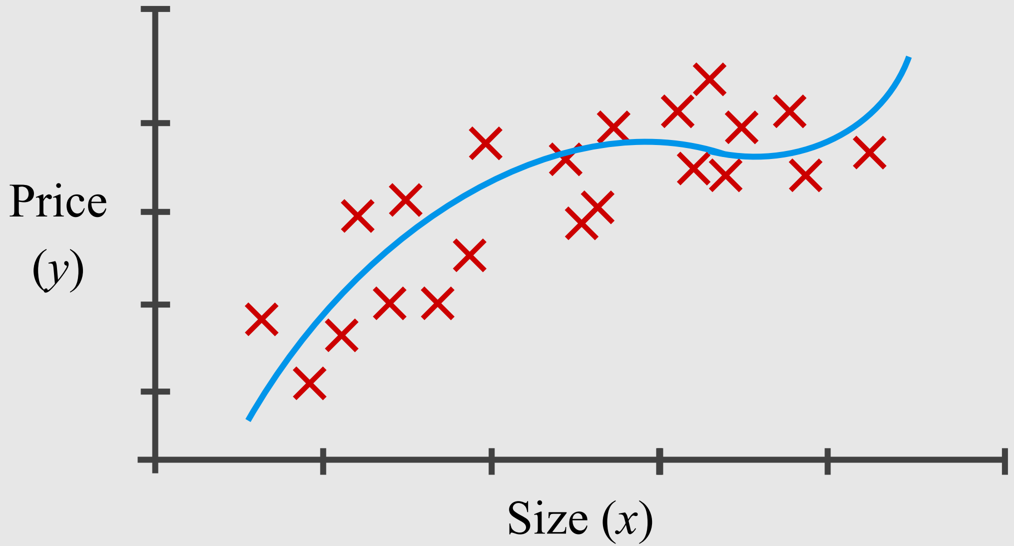
$$x_1 = (\text{size})$$

$$x_2 = (\text{size})^2$$

$$x_3 = (\text{size})^3$$

$$\begin{aligned} h_\theta(x) &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 \\ &= \theta_0 + \theta_1(\text{size}) + \theta_2(\text{size})^2 + \theta_3(\text{size})^3 \end{aligned}$$

Polynomial Regression



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

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

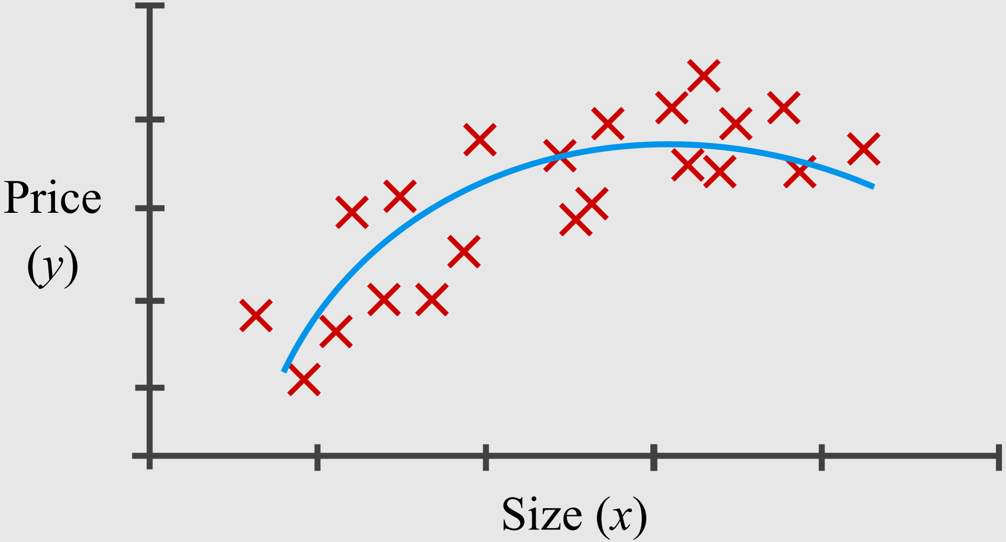
$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
$$= \theta_0 + \theta_1(\text{size}) + \theta_2(\text{size})^2 + \theta_3(\text{size})^3$$

$x_1 = (\text{size})$ $:1\text{–}1{,}000$

$x_2 = (\text{size})^2$ $:1\text{–}1{,}000{,}000$

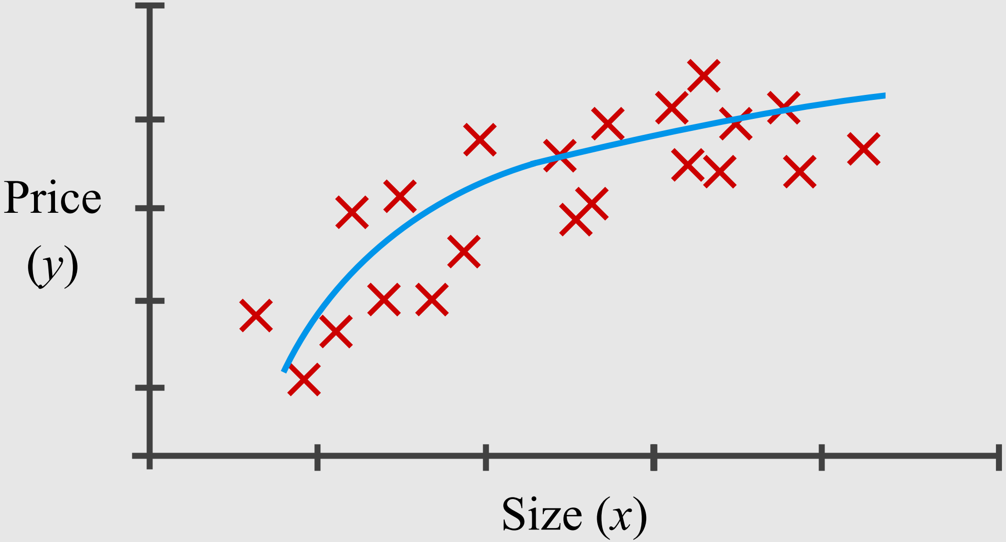
$x_3 = (\text{size})^3$ $:1\text{–}10^9$

Choice of Features



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

Choice of Features

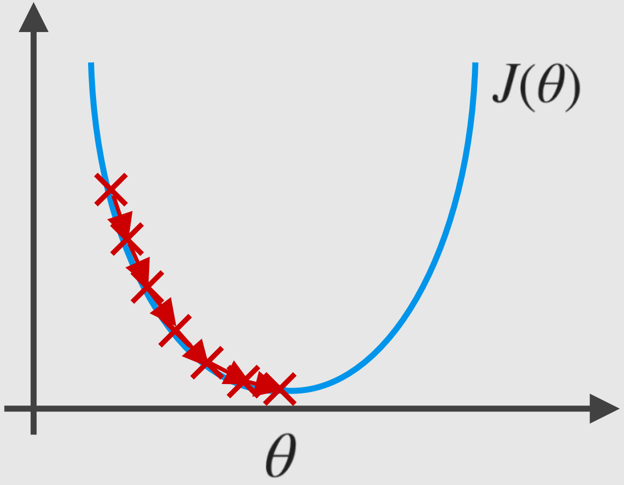


$$h_\theta(x) = \theta_0 + \theta_1(\text{ size }) + \theta_2(\text{ size })^2$$

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

Normal Equation

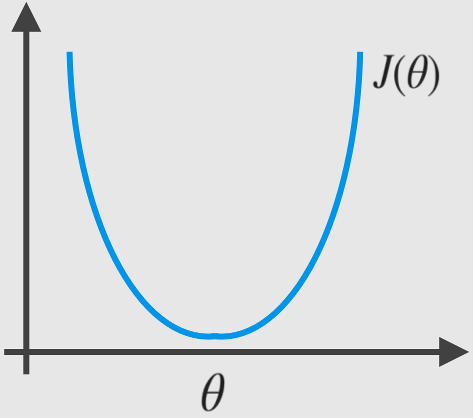
Gradient Descent



Normal equation: Method to solve θ **analytically**.

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

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



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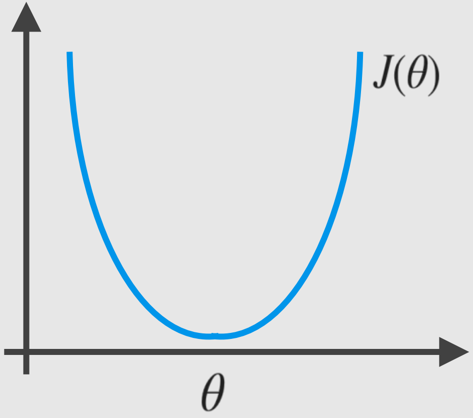
Solve for θ



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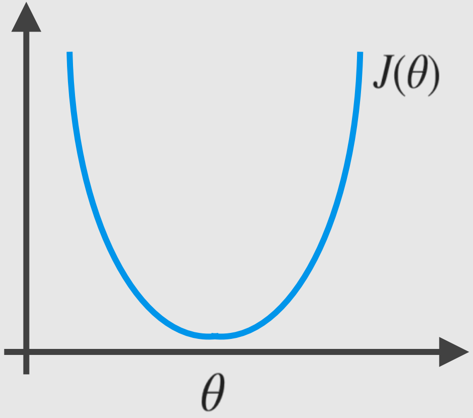

$\theta \in \mathbb{R}^{n+1}$

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

$$\frac{\partial}{\partial \theta_j} J(\theta) = \cdots = 0$$

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

Examples: $m = 4$.

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

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 ($) in 1000's** y
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$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}$$

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

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

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

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

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

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

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

E.g. $x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$

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

E.g. $x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$ $\quad X = \begin{bmatrix} 1 & x_1^{(1)} \\ \vdots & \vdots \\ 1 & x_m^{(1)} \end{bmatrix}_{m \times 2}$

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

$$X = \begin{bmatrix} \text{——} & (x^{(1)})^{\mathrm{T}} & \text{——} \\ \text{——} & (x^{(2)})^{\mathrm{T}} & \text{——} \\ \text{——} & \vdots & \text{——} \\ \text{——} & (x^{(m)})^{\mathrm{T}} & \text{——} \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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

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Deriving the Normal Equation using matrix calculus …

👉 https://ayearofai.com/rohan-3-deriving-the-normal-equation-using-matrix-calculus-1a1b16f65dda

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What if $X^T X$ is noninvertible?

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The common causes might be having :

- Redundant features, where two features are very closely related (i.e. they are linearly dependent).
- Too many features (e.g. $m \leq n$). In this case, delete some features or use "regularization".

Gradient Descent

- 😞 Need to choose α.
- 😞 Needs many iterations.

Normal Equation

- 😃 No need to choose α.
- 😃 Don’t need to iterate.

m examples and n features

Gradient Descent

- 😞 Need to choose α.
- 😞 Needs many iterations.
- 😃 Works well even when n is large.

Normal Equation

- 😃 No need to choose α.
- 😃 Don't need to iterate.
- 😞 Need to compute $(X^T X)^{-1} \rightarrow O(n^3)$.
- 😞 Slow if n is very large.

m examples and n features

References

Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 2 & 4
- Pattern Recognition and Machine Learning, Chap. 3
- Machine Learning: a Probabilistic Perspective, Chap. 7

Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 1 & 2