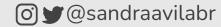


# Linear Regression Machine Learning

(Largely based on slides from Andrew Ng)

### Prof. Sandra Avila

Institute of Computing (IC/Unicamp)



MC886/MO444, August 30, 2022

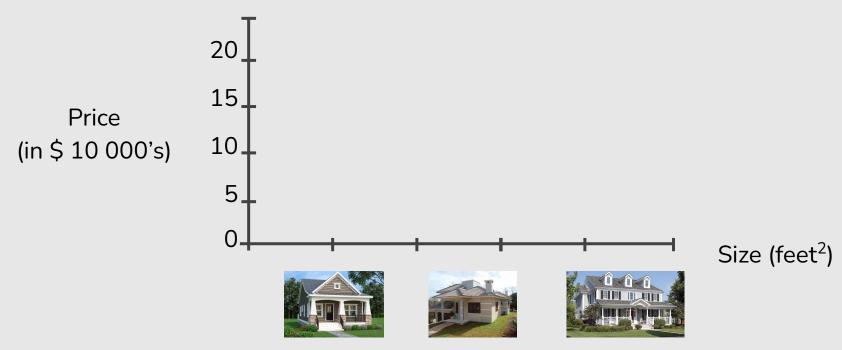


\$ 70 000

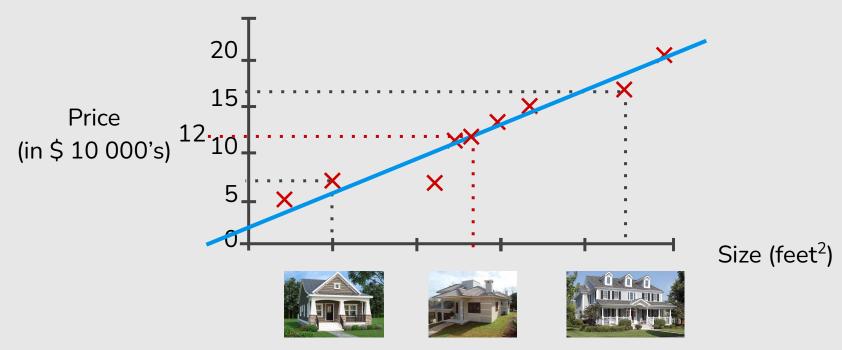


\$ 160 000





### **Linear Regression**







Hom

Competitions

₩ Datasets

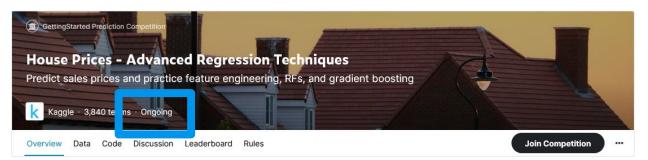
<> Code

Discussions

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More

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#### Description Evaluation

Overview

**Tutorials** 

Frequently Asked Questions

#### Start here if...

You have some experience with R or Python and machine learning basics. This is a perfect competition for data science students who have completed an online course in machine learning and are looking to expand their skill set before trying a featured competition.

#### Competition Description



Ask a home buyer to describe their dream house, and they probably won't begin with the height of the basement ceiling or the proximity to an east-west railroad. But this playground competition's dataset proves that much more influences price negotiations than the number of bedrooms or a white-picket fence.

With 79 explanatory variables describing (almost) every aspect of residential homes in Ames, lowa, this competition challenges you to predict the final price of each home.





Competitions

Datasets

<> Code

Discussions

Courses

✓ More

Q Search





C Refresh

Q Search leaderboard

This leaderboard is calculated with all of the test data.

#	Team	Members	Score	Entries	Last	Code	Join
1	fedesoriano		0.00000	2	23d		
2	Lev1nLee	<b></b>	0.00000	1	2d		
3	Moshi Wei	4)	0.00044	3	2mo		
4	Jewel Liu		0.00044	1	2mo		
5	YIYANG HAO		0.00044	13	6d		
6	Bing Guo	(4)	0.00044	4	2mo		

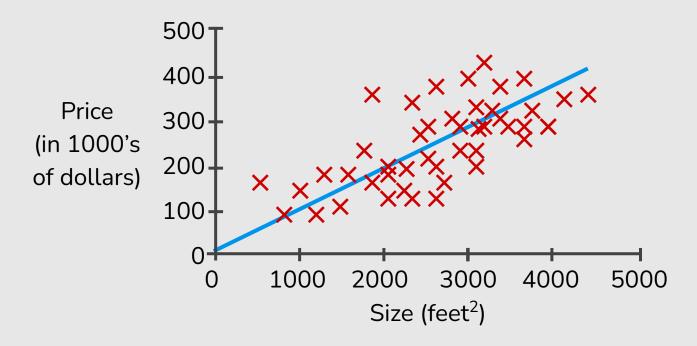
### Today's Agenda

\_ \_ \_

- 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

### **Housing Prices**



### **Supervised Learning**

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

### Regression Problem

Predict real-valued output

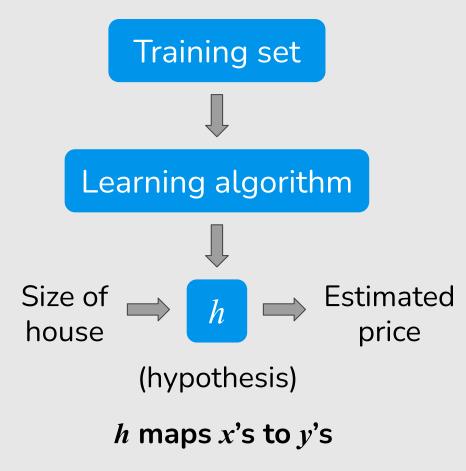
Training	set of
housing	prices

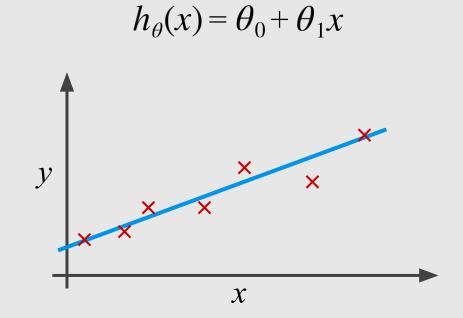
Size in feet <sup>2</sup> (x)	Price (\$) in 1000's (y)		
2104	460		
1416	232		
1534	315		
852	178		
•••	•••		

#### Notation:

m = Number of training examplesx's = "input" variable / featuresy's = "output" variable / "target" variable

### How do we represent h?





Linear regression with one variable.

Univariate linear regression.

### Cost Function

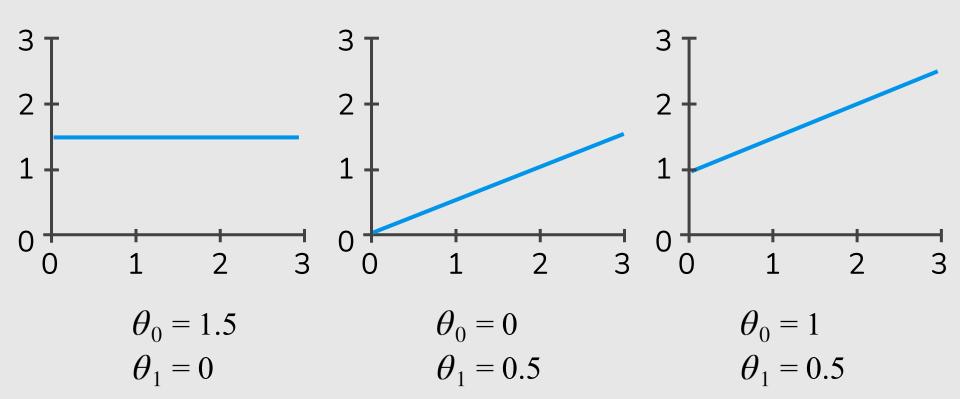
Training Set	Size in feet <sup>2</sup> (x)	Price (\$) in 1000's (y)
	2104	460
	1416	232
	1534	315
	852	178

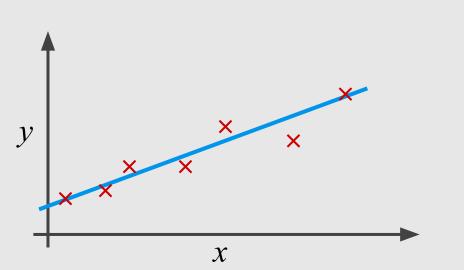
Hypothesis:  $h_{\theta}(x) = \theta_0 + \theta_1 x$ 

 $\theta i$ 's: Parameters

How to choose  $\theta i$ 's?

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





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

$$h_{\theta}(x) = \theta_{0} + \theta_{1}x$$

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

Choose  $\theta_0$ ,  $\theta_1$  so that  $h_{\theta}(x)$  close to y for our training examples (x,y)

$$\begin{array}{c}
\text{minimize } J(\theta_0, \theta_1) \\
\theta_0, \theta_1
\end{array}$$

Cost function (Squared error function) 17

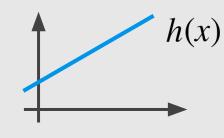
# Cost Function Intuition I

### **Hypothesis:**

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

#### **Parameters:**

$$\theta_0, \theta_1$$



#### **Cost Function:**

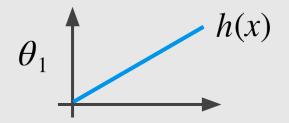
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

#### Goal:

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

### **Simplified**

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



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

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

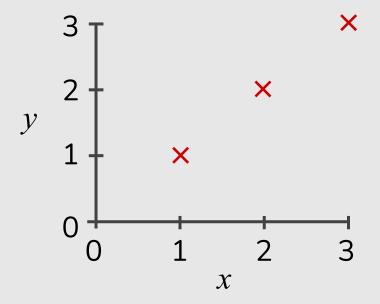
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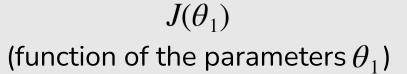
(for fixed  $\theta_1$ , this is a function of x)

$$J(\theta_1)$$

(function of the parameters  $\theta_1$ )

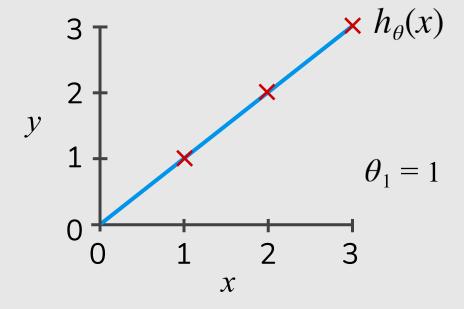
# $h_{\theta}(x)$ (for fixed $\theta_1$ , this is a function of x)





### $h_{\theta}(x)$

(for fixed  $\theta_1$ , this is a function of x)



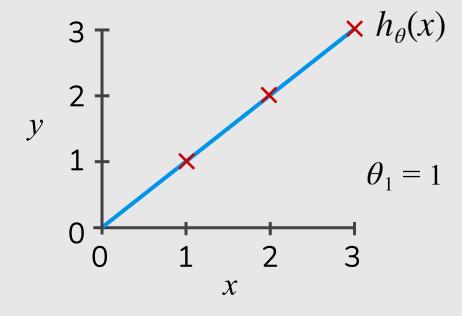
 $J(\theta_1) = J(1) = ?$ 

$$J( heta_1)$$

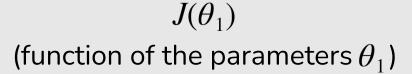
(function of the parameters  $\theta_1$ )

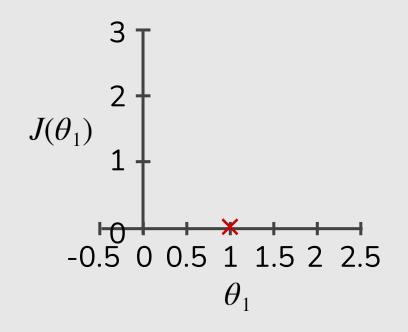
### $h_{\theta}(x)$

(for fixed  $\theta_1$ , this is a function of x)

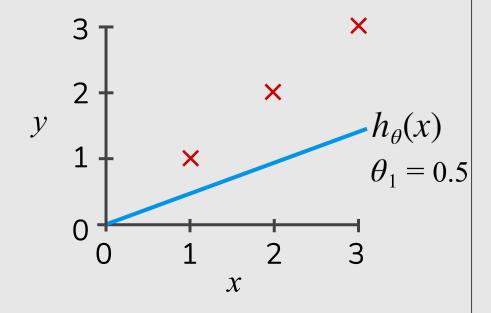


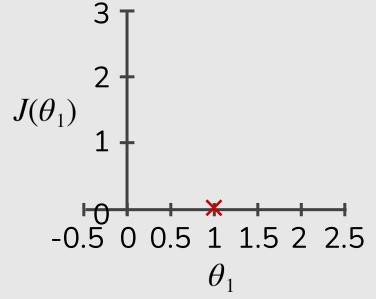
$$J(\theta_1) = J(1) = 0$$



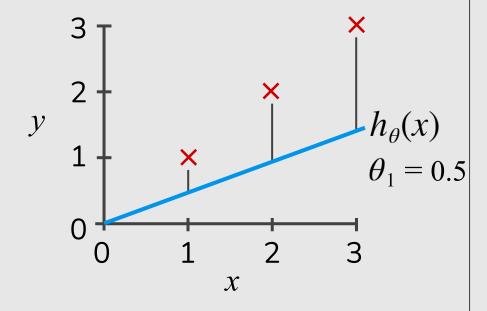


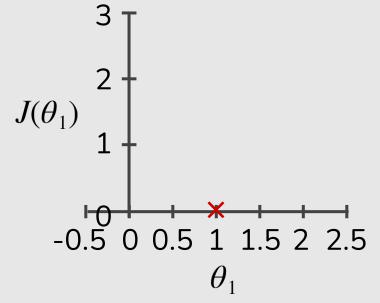
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



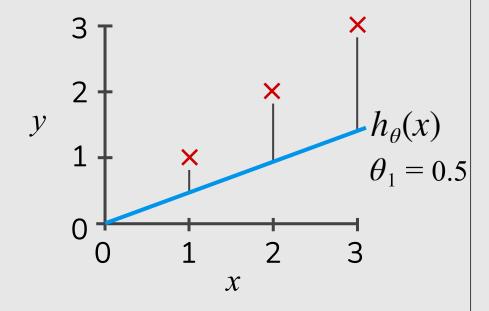


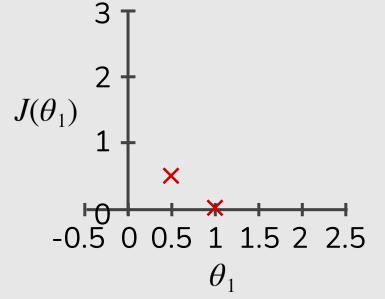
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



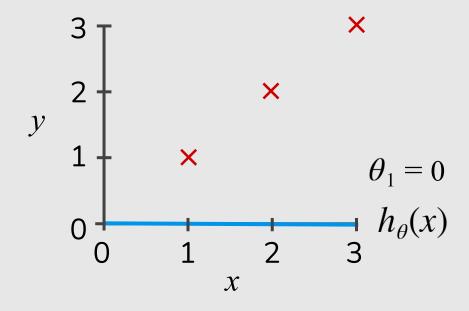


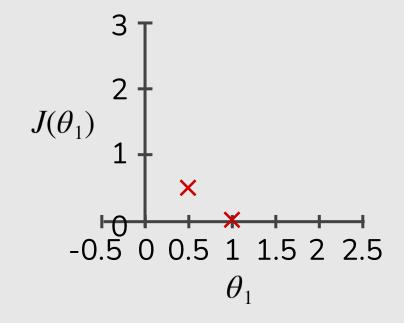
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



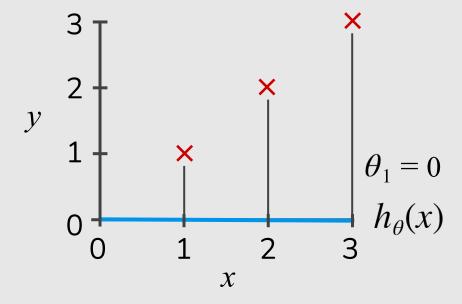


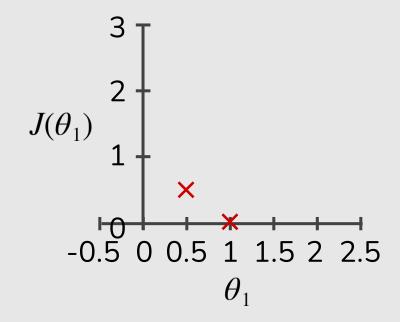
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



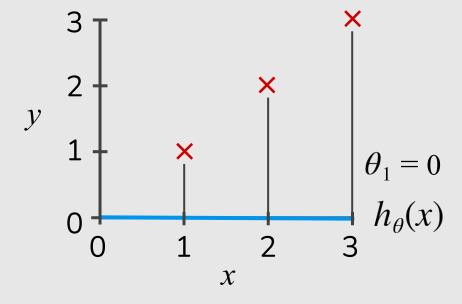


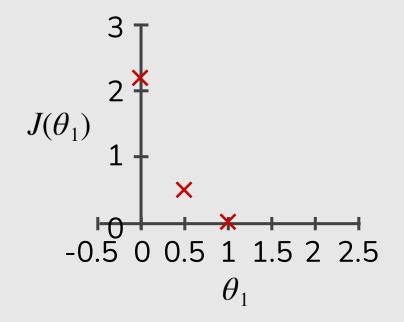
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



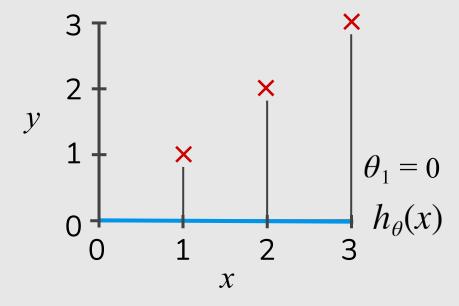


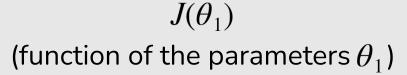
 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)

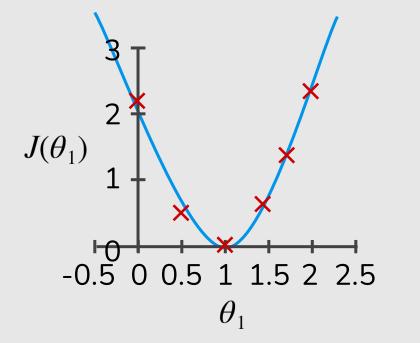




 $h_{\theta}(x)$  (for fixed  $\theta_1$ , this is a function of x)



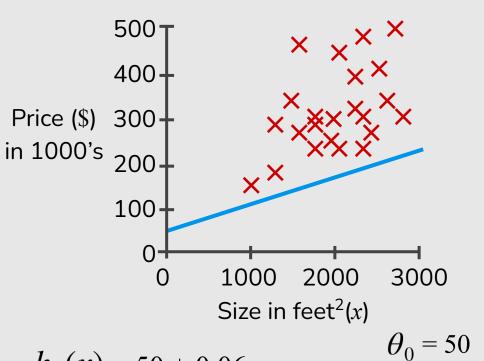




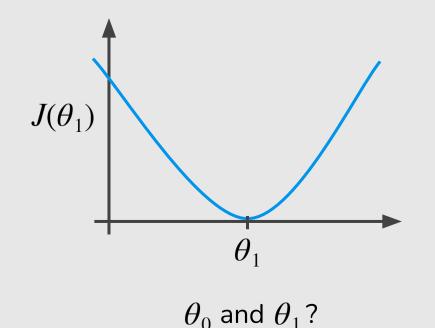
# Cost Function Intuition II

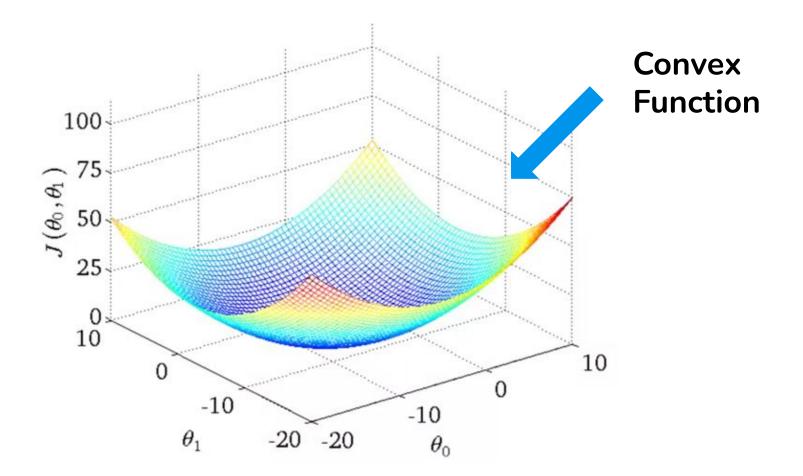
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)

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

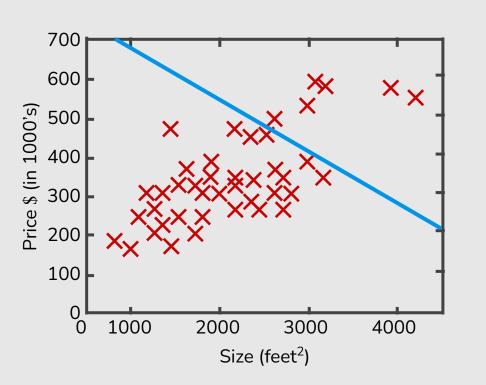


 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\,\theta_1$ )

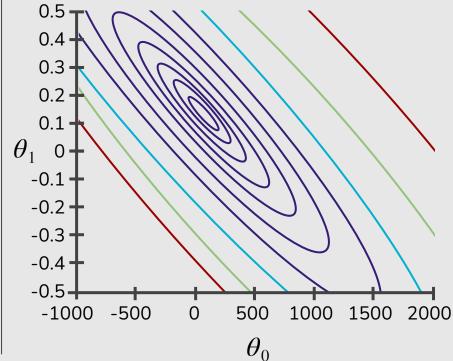




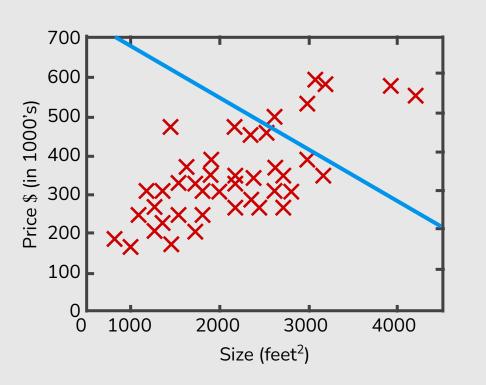
 $h_{\theta}(x)$  (for fixed  $\theta_0, \theta_1$  , this is a function of x)



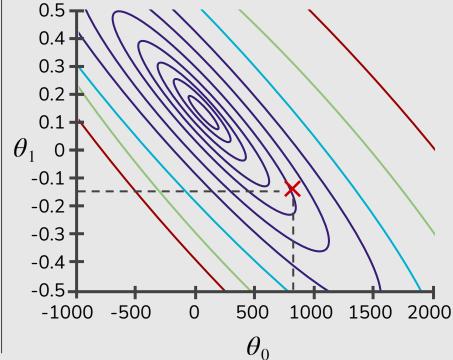
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



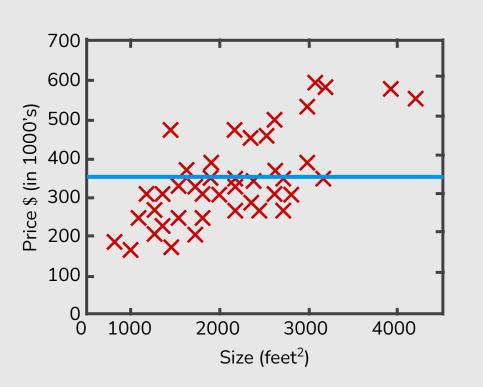
 $h_{\theta}(x)$  (for fixed  $\theta_0, \theta_1$  , this is a function of x)



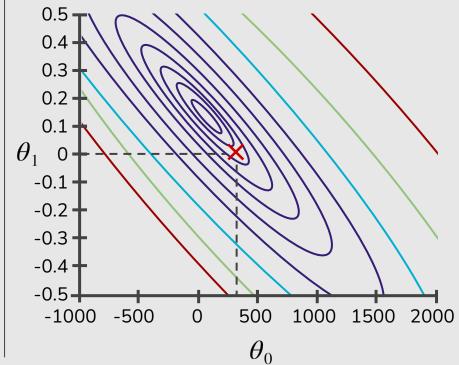
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



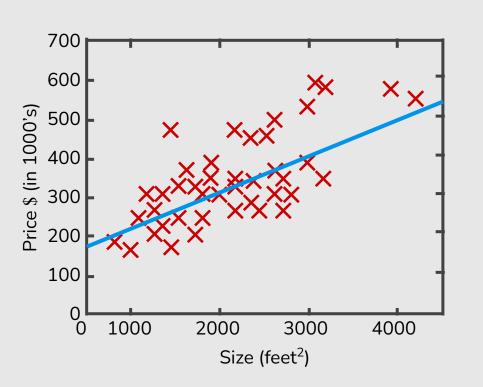
 $h_{\theta}(x)$  (for fixed  $\theta_0, \theta_1$  , this is a function of x)



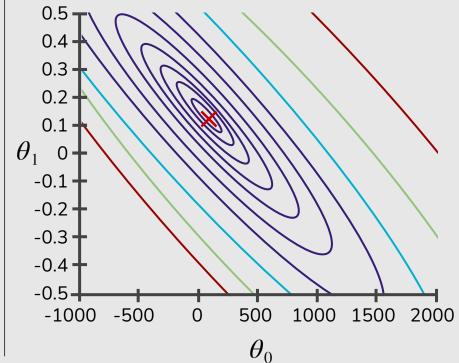
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



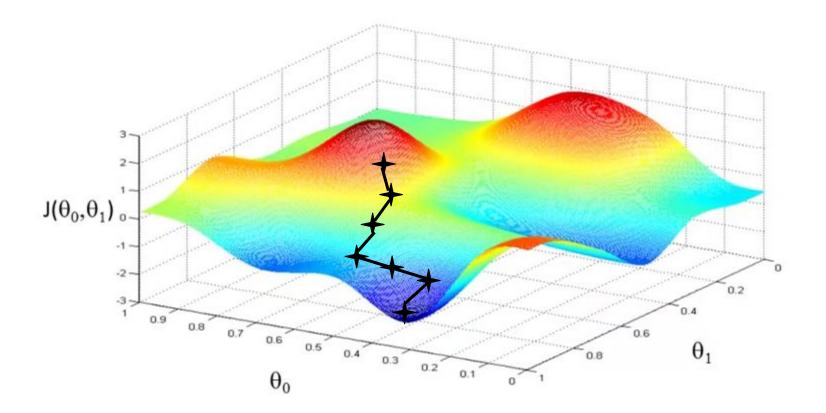
## Gradient Descent

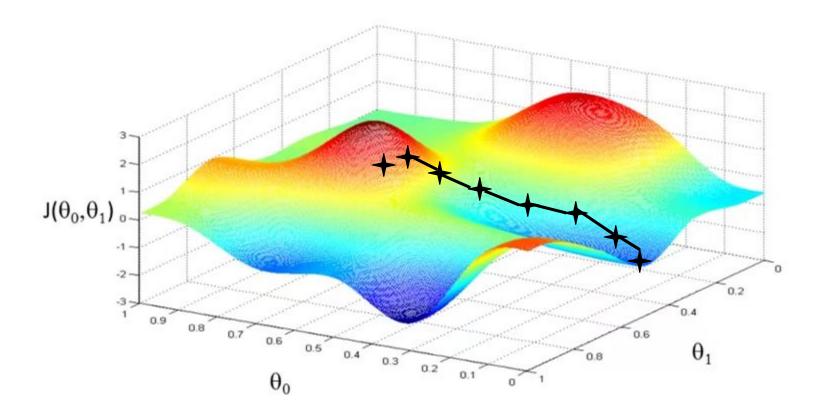
Have some function  $J(\theta_0, \theta_1)$ 

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

#### **Outline:**

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

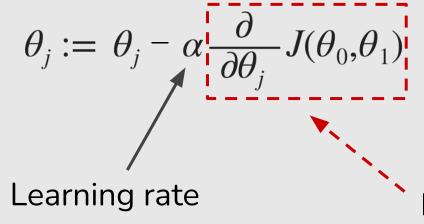




repeat until convergence {

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

repeat until convergence {



(simultaneously update

$$j = 0 \text{ and } j = 1$$
)

Derivative term

repeat until convergence {

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

### Correct: Simultaneous update

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

repeat until convergence {

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

Correct: Simultaneous update

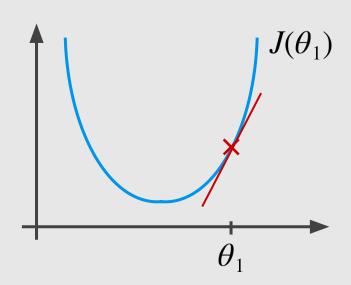
$$\begin{aligned} & \operatorname{temp0} := \, \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\ & \operatorname{temp1} := \, \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\ & \theta_0 := \, \operatorname{temp0} \\ & \theta_1 := \, \operatorname{temp1} \end{aligned}$$

Incorrect

$$\begin{aligned} & \operatorname{temp0} := \, \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\ & \theta_0 := \operatorname{temp0} \\ & \operatorname{temp1} := \, \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\ & \theta_1 := \operatorname{temp1} \end{aligned}$$

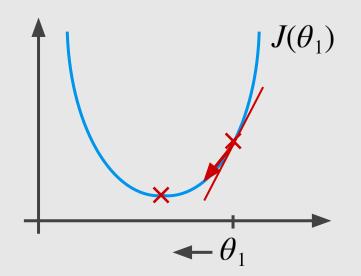
$$\theta_1 := \text{temp}$$

 $\theta_1 \subseteq \mathbb{R}$ 



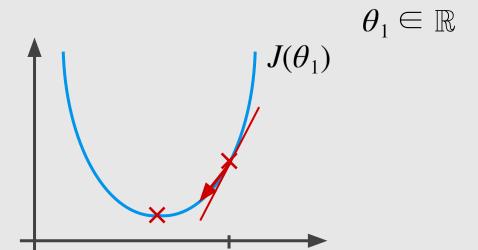
$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

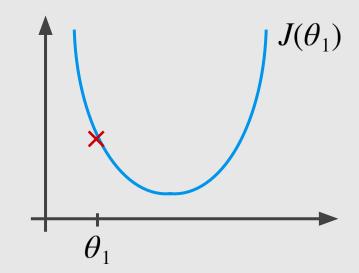




$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

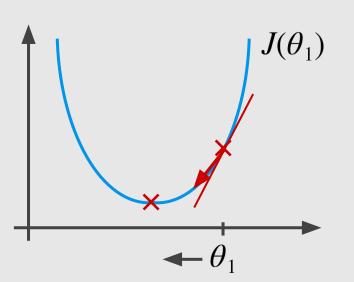
$$\theta_1 := \theta_1 - \alpha \cdot \text{(positive number)}$$



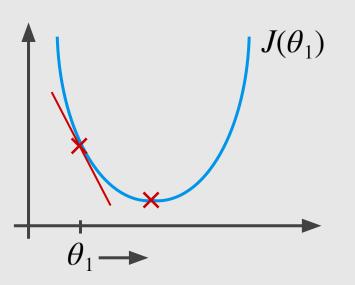


$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$
  $\geq 0$ 

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



$$\theta_1 \subseteq \mathbb{R}$$



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

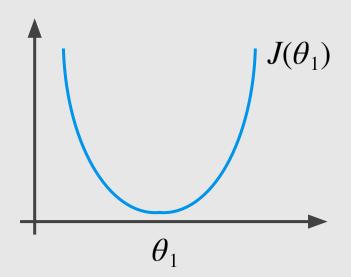
$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

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

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

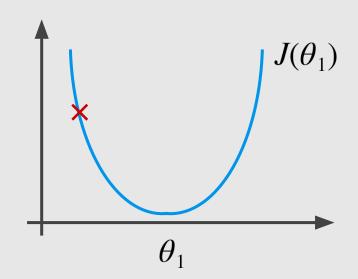
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If  $\alpha$  is too small, gradient descent can be ...



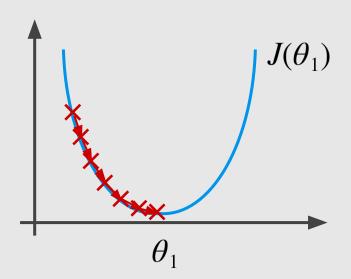
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If  $\alpha$  is too small, gradient descent can be ...



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

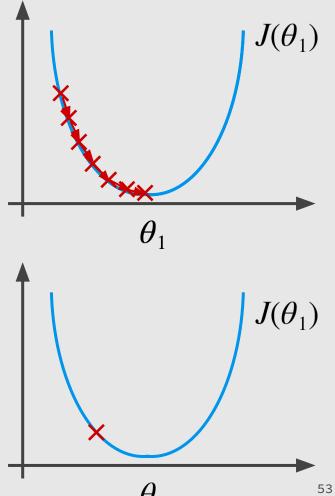
If  $\alpha$  is too small, gradient descent can be slow.



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

If  $\alpha$  is too small, gradient descent can be slow.

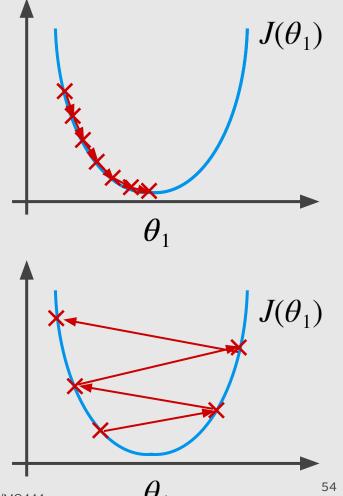
If  $\alpha$  is too large, gradient descent can be ...



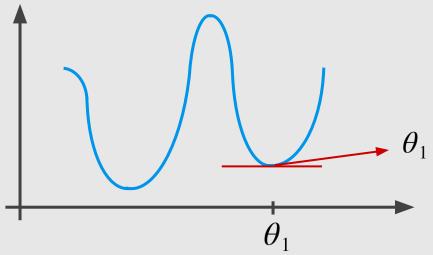
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If  $\alpha$  is too small, gradient descent can be slow.

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



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



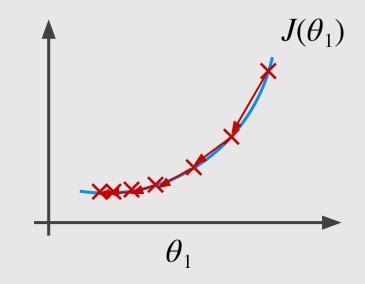
$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

 $\theta_1$  at local optima

Gradient descent can converge to a local minimum, even with the learning rate  $\alpha$  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  $\alpha$  over time.



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**

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

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

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

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

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

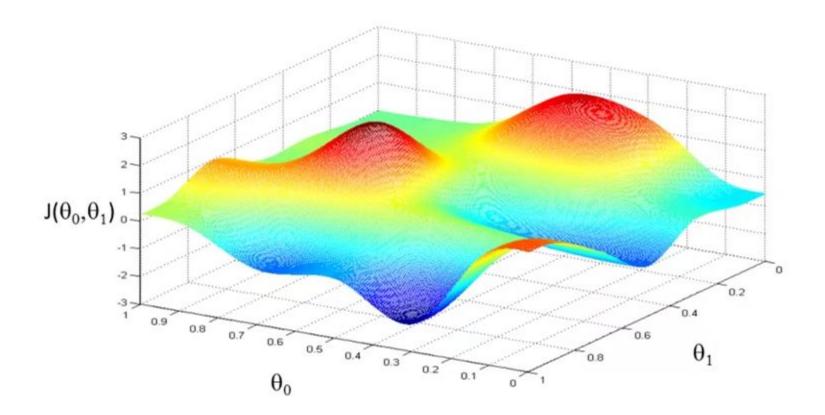
$$= \frac{1}{\partial \theta_j} \cdot \frac{1}{2m} \sum_{i=1}^{m} (\theta_0 + \theta_1 x^{-1} - y^{-1})$$

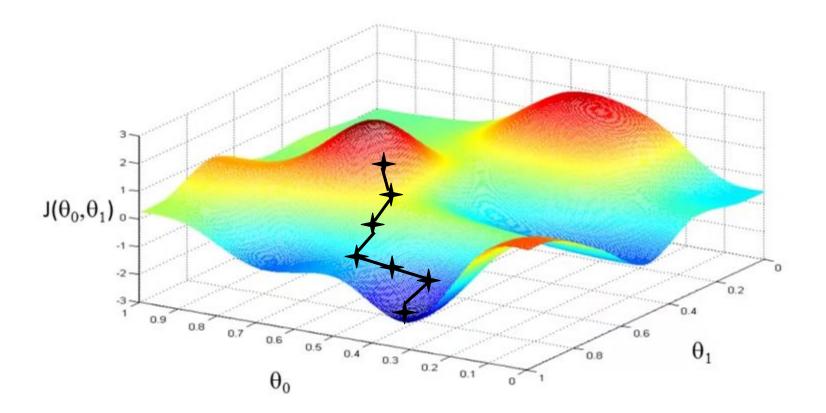
$$j = 0$$
:  $\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})$ 

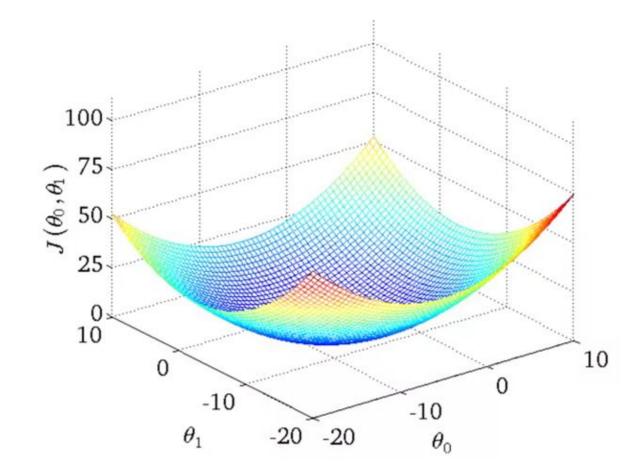
$$j = 1$$
:  $\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) x^{(i)}$ 

repeat until convergence {

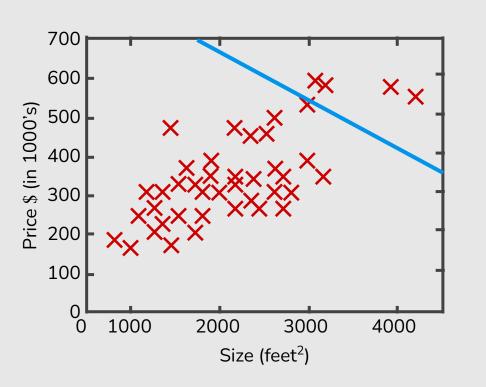
$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})$$
 
$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x^{(i)}$$
 update  $\theta_0$  and  $\theta_1$  simultaneously



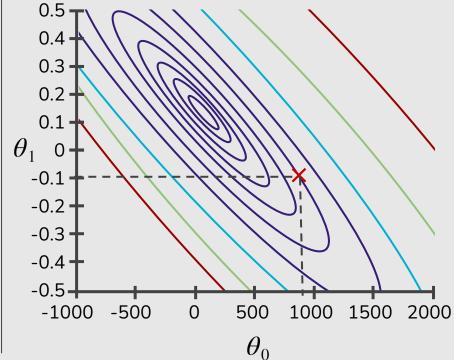




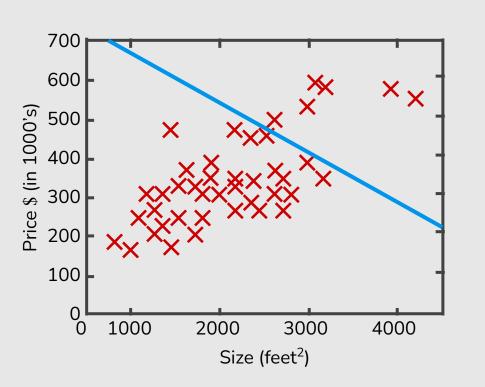
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



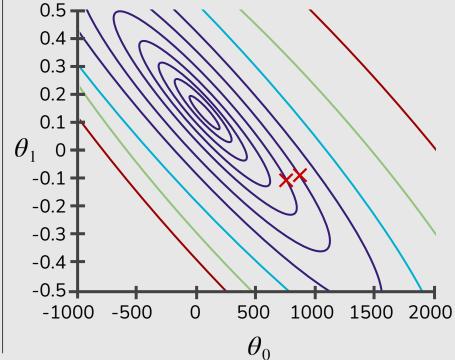
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



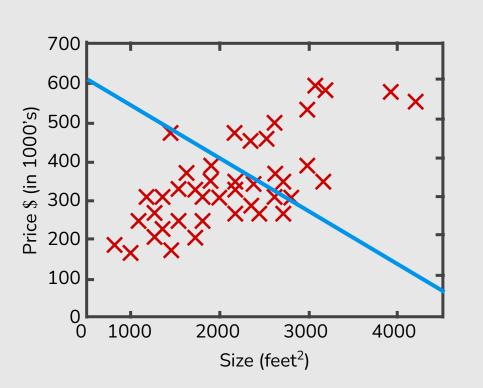
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



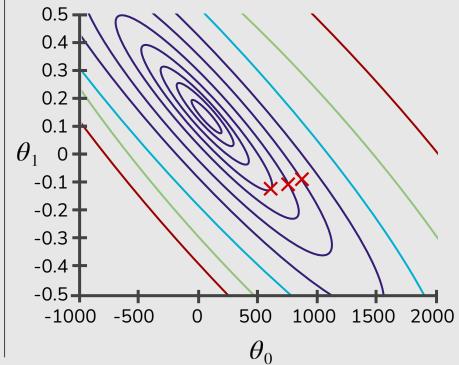
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



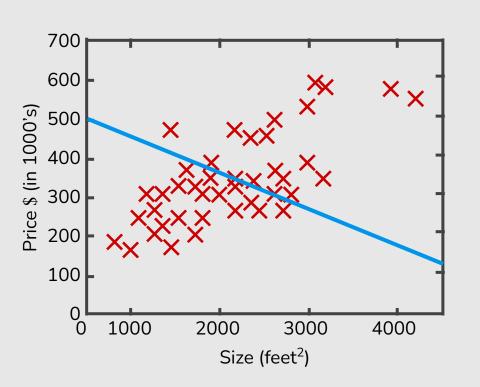
 $h_{\theta}(x)$  (for fixed  $\theta_0, \theta_1$  , this is a function of x)



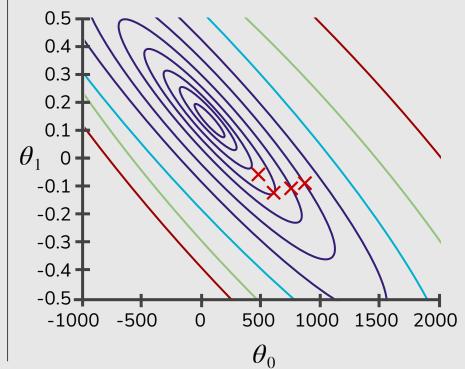
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



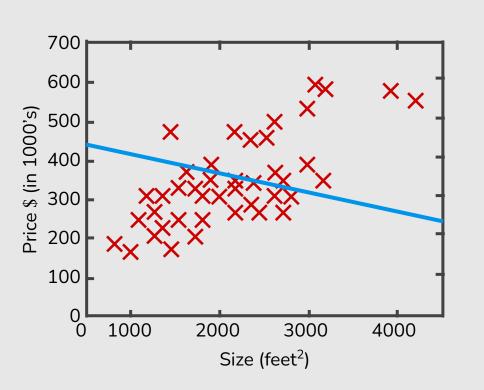
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



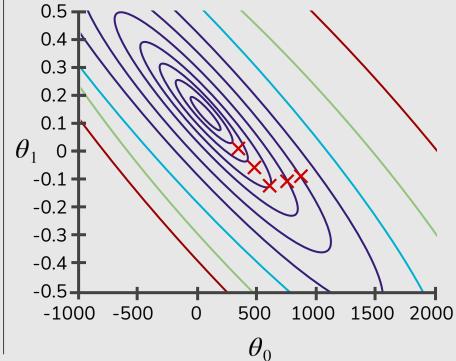
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



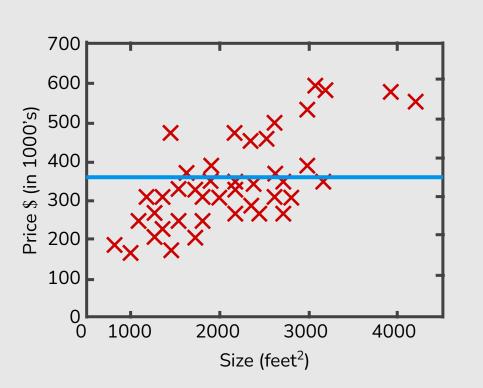
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



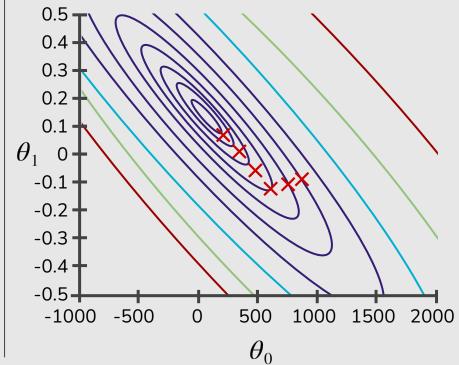
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



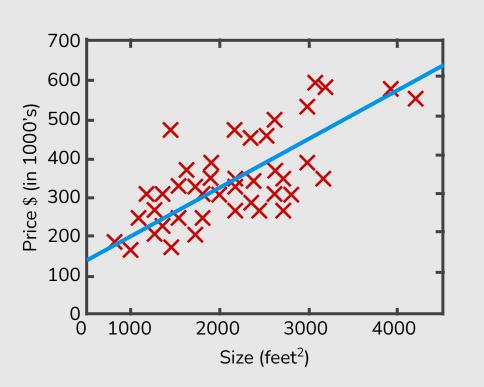
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



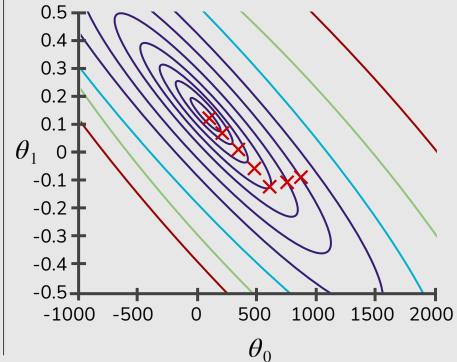
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )



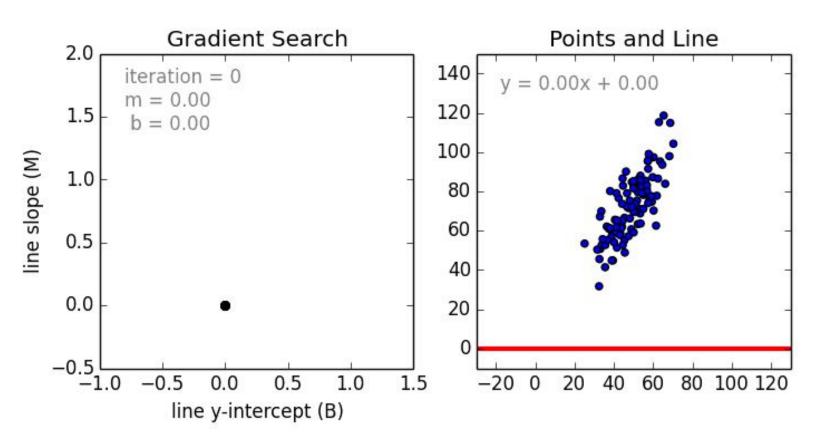
 $h_{\theta}(x)$  (for fixed  $\theta_0$ ,  $\theta_1$ , this is a function of x)



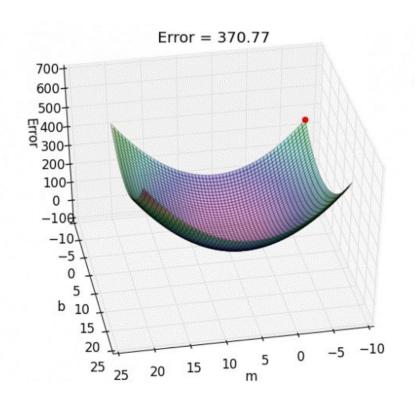
 $J(\theta_0,\!\theta_1)$  (function of the parameters  $\theta_0,\!\theta_1$  )

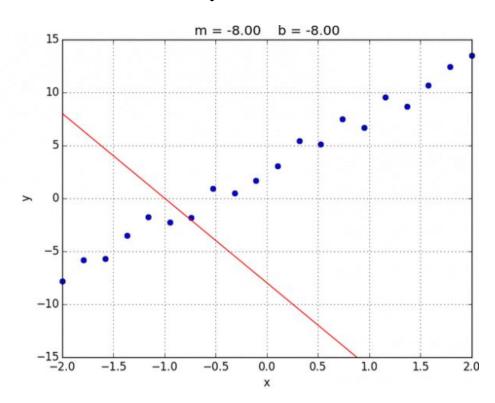


$$h_{\theta}(x) = \theta_0 + \theta_1 x \implies y = b + mx$$



$$y = b + mx$$





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.

- 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  $\theta_0$  and  $\theta_1$  simultaneously

}

## Stochastic Gradient Descent

Each step of gradient descent uses one training example.

```
repeat until convergence {
```

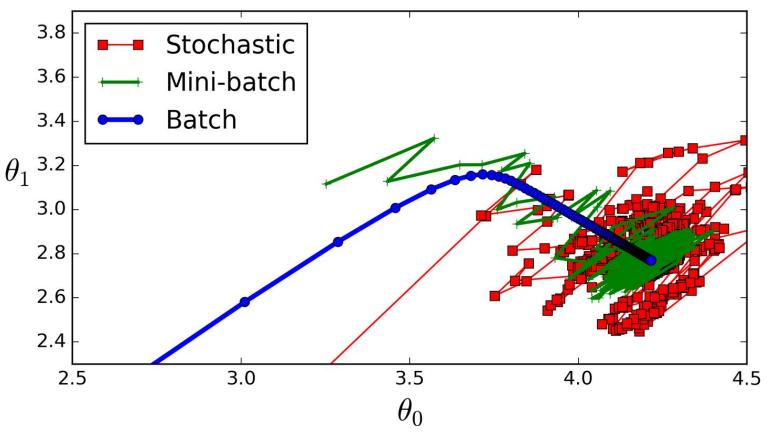
```
for i = 1, ..., m { \theta_0 := \theta_0 - \alpha(h_\theta(x^{(i)}) - y^{(i)}) \theta_1 := \theta_1 - \alpha(h_\theta(x^{(i)}) - y^{(i)})x^{(i)} }
```

## Mini-batch Gradient Descent

Each step of gradient descent uses b training examples.

```
Say b = 10, m = 1000.
repeat until convergence {
      for i = 1, 11, 21..., 991 {
             \theta_0 := \theta_0 - \alpha \frac{1}{10} \sum_{k=0}^{i+9} (h_{\theta}(x^{(k)}) - y^{(k)})
             \theta_1 := \theta_1 - \alpha \frac{1}{10} \sum_{i+9}^{i=k} (h_{\theta}(x^{(k)}) - y^{(k)}) x^{(k)}
```

## Batch vs. Stochastic vs. Mini-batch



## References

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#### **Machine Learning Books**

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 2 & 4
- Pattern Recognition and Machine Learning, Chap. 3
- Probabilistic Machine Learning: An Introduction, Chap. 11

## References

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#### **Machine Learning Courses**

- https://www.coursera.org/learn/machine-learning, Week 1 & 2
- https://ml-cheatsheet.readthedocs.io/en/latest/linear\_regression.html

#### **Machine Learning Videos**

- Linear Regression: A friendly introduction, <a href="https://youtu.be/wYPUhge9w5c">https://youtu.be/wYPUhge9w5c</a>
- Linear Regression, Clearly Explained!!!, <a href="https://youtu.be/nk2CQITm\_eo">https://youtu.be/nk2CQITm\_eo</a>

## 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