Machine Learning

Linear Regression

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Acknowledgement:
This lecture is based on (but not limited to) Andrew Ng's course about Machine Learning
https://www.youtube.com/channel/UCMoXOGX9mgrYNEwpcIQUcag

Machine Learning
Linear Regression

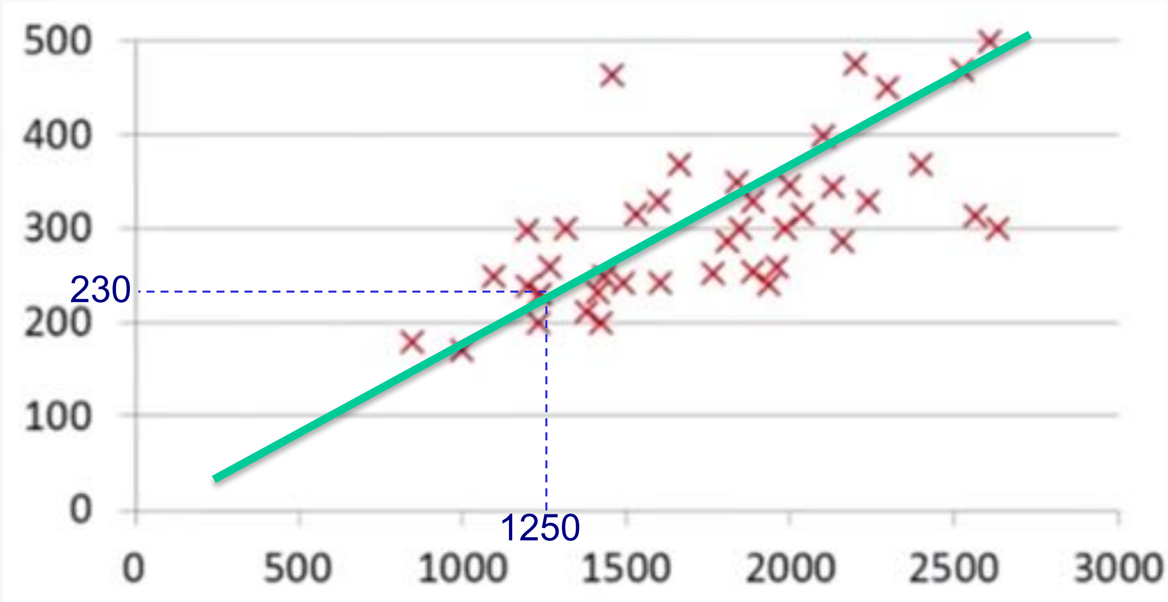
In this lecture:

- Part 1: **Motivation (Regression Problems)**
- Part 2: Linear Regression
- Part 3: The Cost Function
- Part 4: The Gradient Descent Algorithm
- Part 5: The Normal Equation
- Part 6: Linear Algebra overview
- Part 7: Using Octave
- Part 8: Using R

Motivation

Given the following **housing prices,**

Price
(in 1000s
of dollars)



Size (feet^2)

How much a house of 1250ft^2 costs?

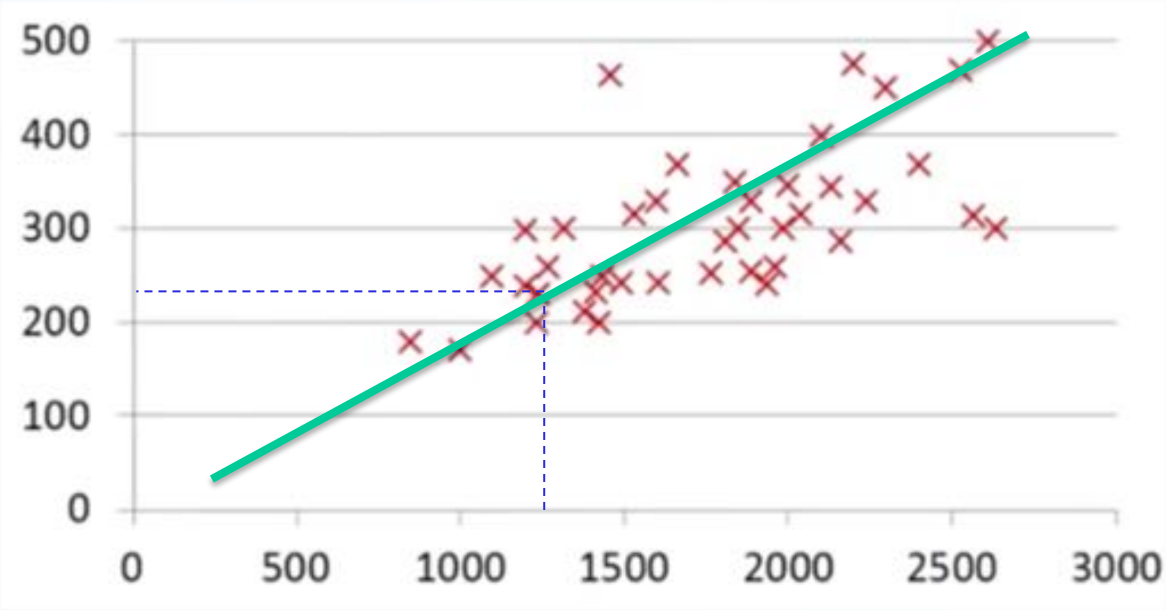
We may assume a linear curve,

So, conclude that a house with 1250ft^2 costs 230K$.

Motivation

Given the following **housing prices**

Price
(in 1000s
of dollars)



Size (feet^2)

Supervised Learning:

Given the right answers for each example in the data (training data)

Regression Problem:

Predict real-valued output

Remember that classification (not regression) refers to predicting discrete-valued output

Motivation

Given the following **training set** of housing prices:

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

Our job is to learn from this data how to predict prices

Notation:

m = Number of training examples

x's = "input" variable/features

y's = output variable/target variable

(x, y) : a training example

(x^i, y^i) : the i^{th} training example

For example:

$x^1 = 2104$

$y^1 = 460$

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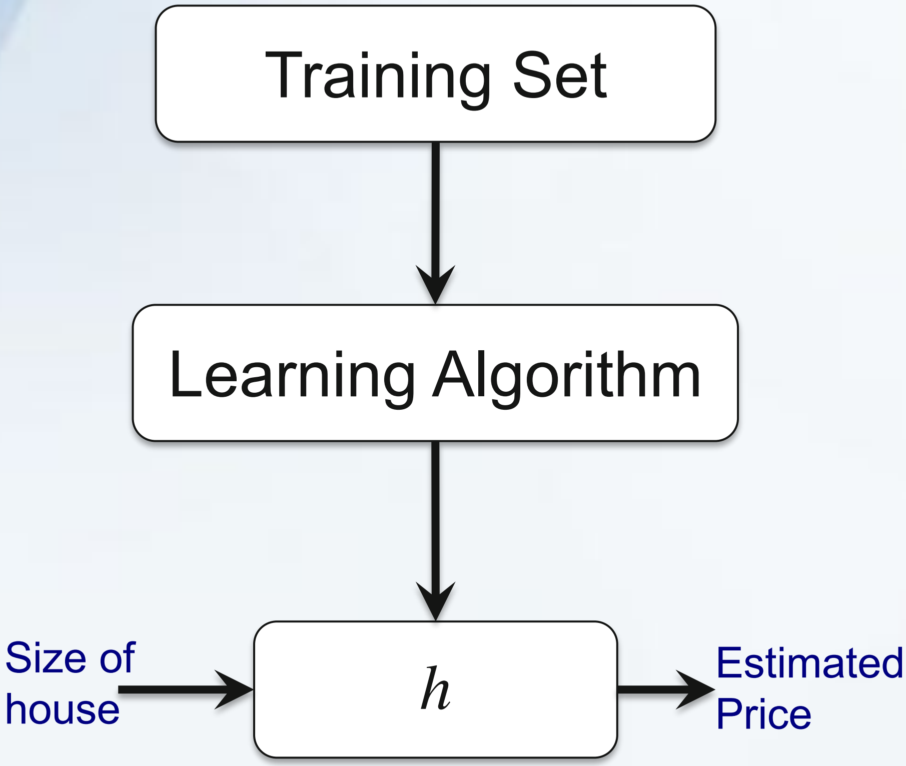
Linear Regression

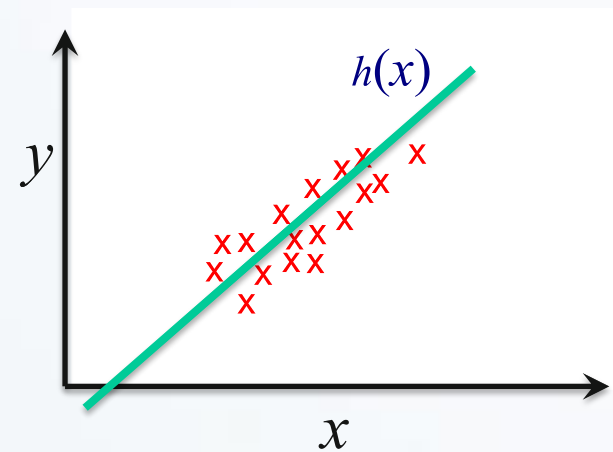


Hypothesis

h maps x's to y's

How to represent h?

$$h(x) = \theta_0 + \theta_1 x$$



- This is a linear function.
- Also called linear regression with one variable.

Linear Regression with Multiple Features

Linear regression with multiple features is also called *multiple linear regression*

Suppose we have the following features

x_1 Size ft²	x_2 bedrooms	x_3 floors	x_4 Age	y Price
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

A hypothesis function $h(x)$ might be:

$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \ldots + \theta_n x_n$$

or $$h(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \ldots + \theta_n x_n \qquad (x_0 = 1)$$

e.g., $h(x) = 80 + 0.1 \cdot x_1 + 0.01 \cdot x_2 + 3 \cdot x_3 - 2 \cdot x_4$

Polynomial Regression

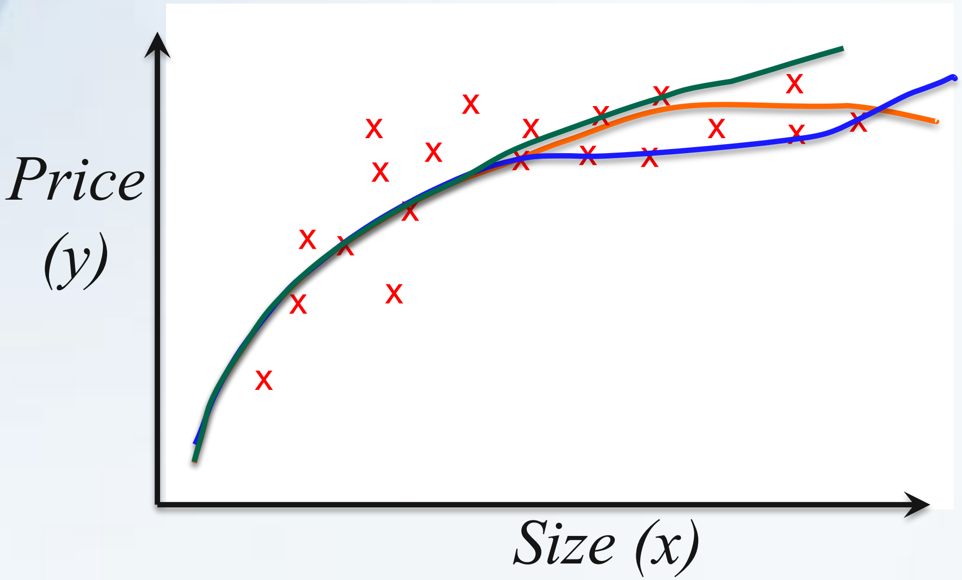
Suppose we have the following features

x_1 Size ft^2	x_2 bedrooms	x_3 floors	x_4 Age	y Price
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

Another hypothesis function $h(x)$ might be (*polynomial*):

$$h(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2^2 + \theta_2 x_3^3 + \ldots + \theta_n x_n^n \qquad (x_0 = 1)$$

Polynomial Regression



$$h(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

$$h(x) = \theta_0 + \theta_1 x + \theta_2 \sqrt[2]{x}$$

$$h(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$

- We may combine features (e.g., size = width * depth).
- We have the option of what features and what models (quadric, cubic,…) to use.
- Deciding which features and models that best fit our data and application, is beyond the scope of this course, but there are several algorithms for this.

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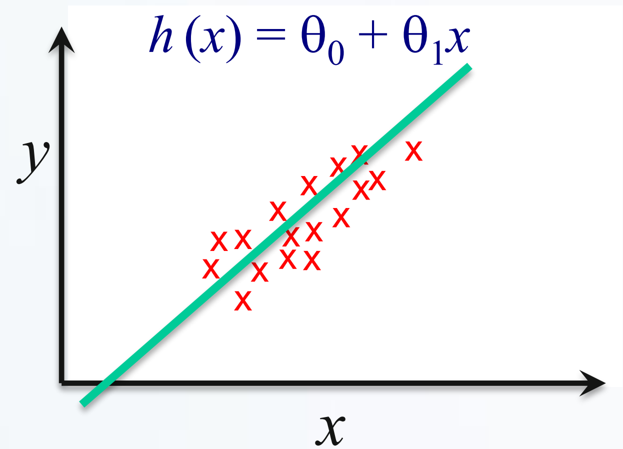
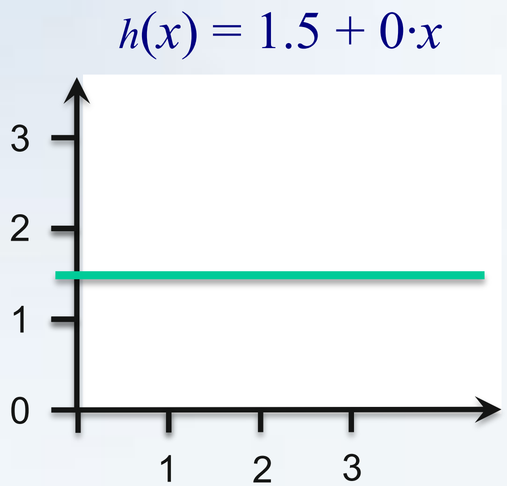
Understanding θs Values

θ_i's: Parameters

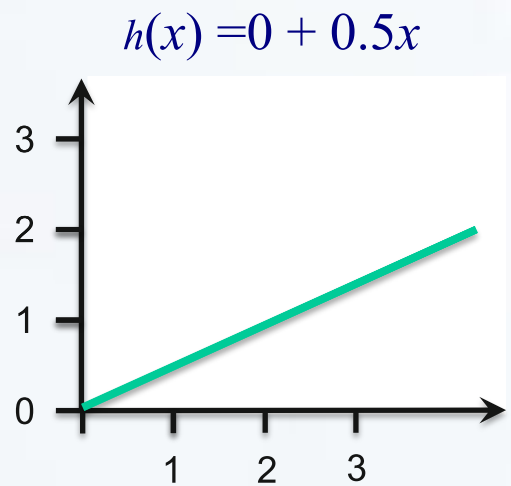
How to choose θ_i's?



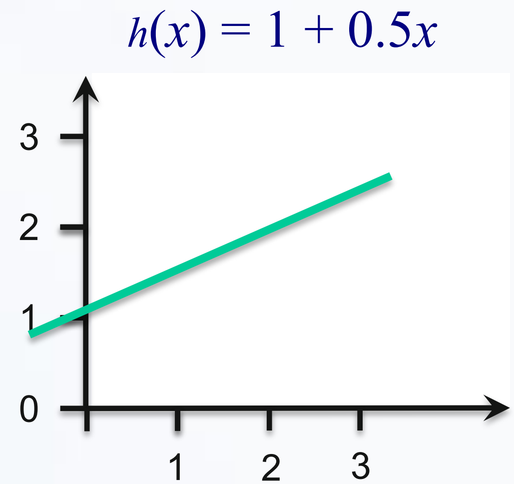
Understanding θs Values



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

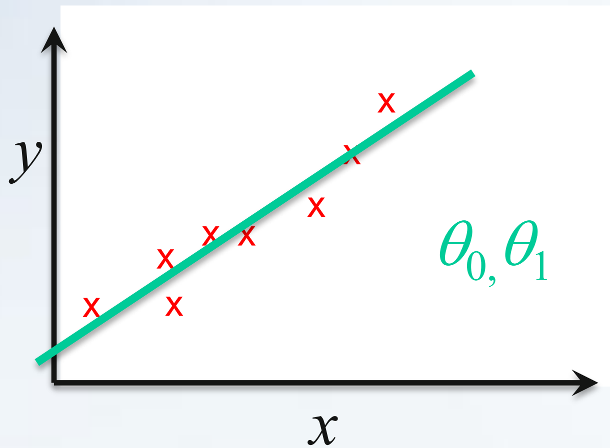


$\theta_0 = 0$
$\theta_1 = 0.5$



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

The Cost Function



Idea: Choose $\theta_{0,} \theta_1$ so that $h(x)$ is close to y for our training examples (x,y).

***y**: is the actual value.*
***h(x)**: is the estimated value.*

The **Cost Function *J*** aims to find θ_0, θ_1 that minimizes the error.

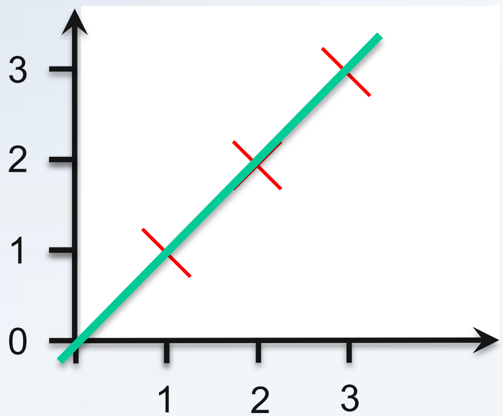
$$J(\theta_{0,} \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h(x^i) - y^i)^2$$

This cost function is also called a **Squared Error function**

Undersetting the Cost Function

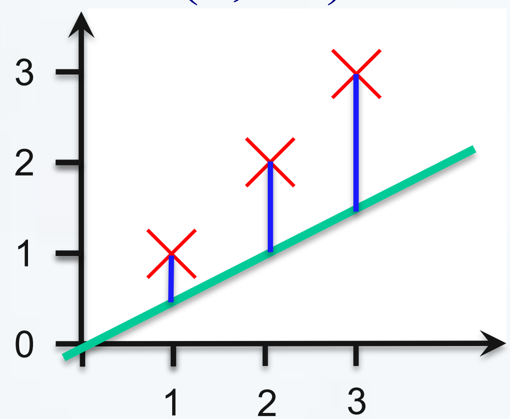
Lets try different values of θs and see how the cost function $J(\theta_{0,}\theta_1)$ behave!

$J(0,1)$



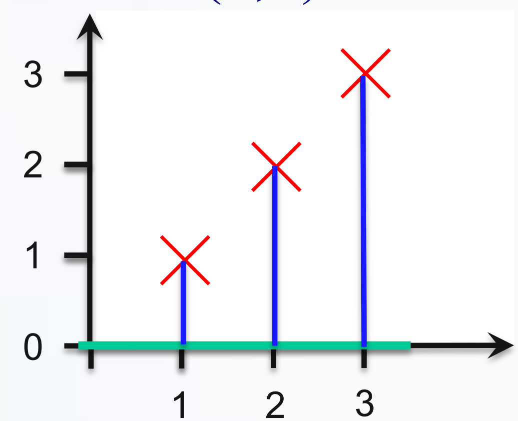
$J(1)= 1/2\cdot3\ [(0)^2+(0)^2(0)^2]$
$= 0$

$J(0,0.5)$



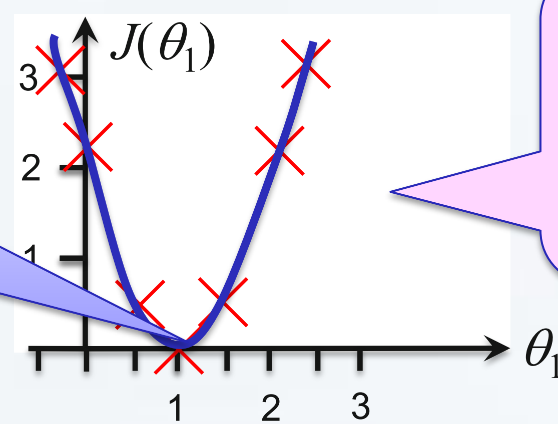
$J(0.5)= 1/2\cdot3\ [(0.5\text{-}1)^2+(1\text{-}2)^2(1.5\text{-}3)^2]$
$\simeq 0.68$

$J(0,0)$



$J(0)= 1/2\cdot3\ [(1)^2+(2)^2(3)^2]$
$\simeq 2.3$

Given our training data, this is the best value of θ_1.



But this figure plots only θ_1, the problem becomes complicated if we have also $(\theta_{0.}\ \theta_{1})$

Cost Function Intuition II

Remember that our goal is find the minimum values of θ_0 and θ_1

Hypothesis: $h(x) = \theta_0 + \theta_1$

Parameters: $\theta_0,\ \theta_1$

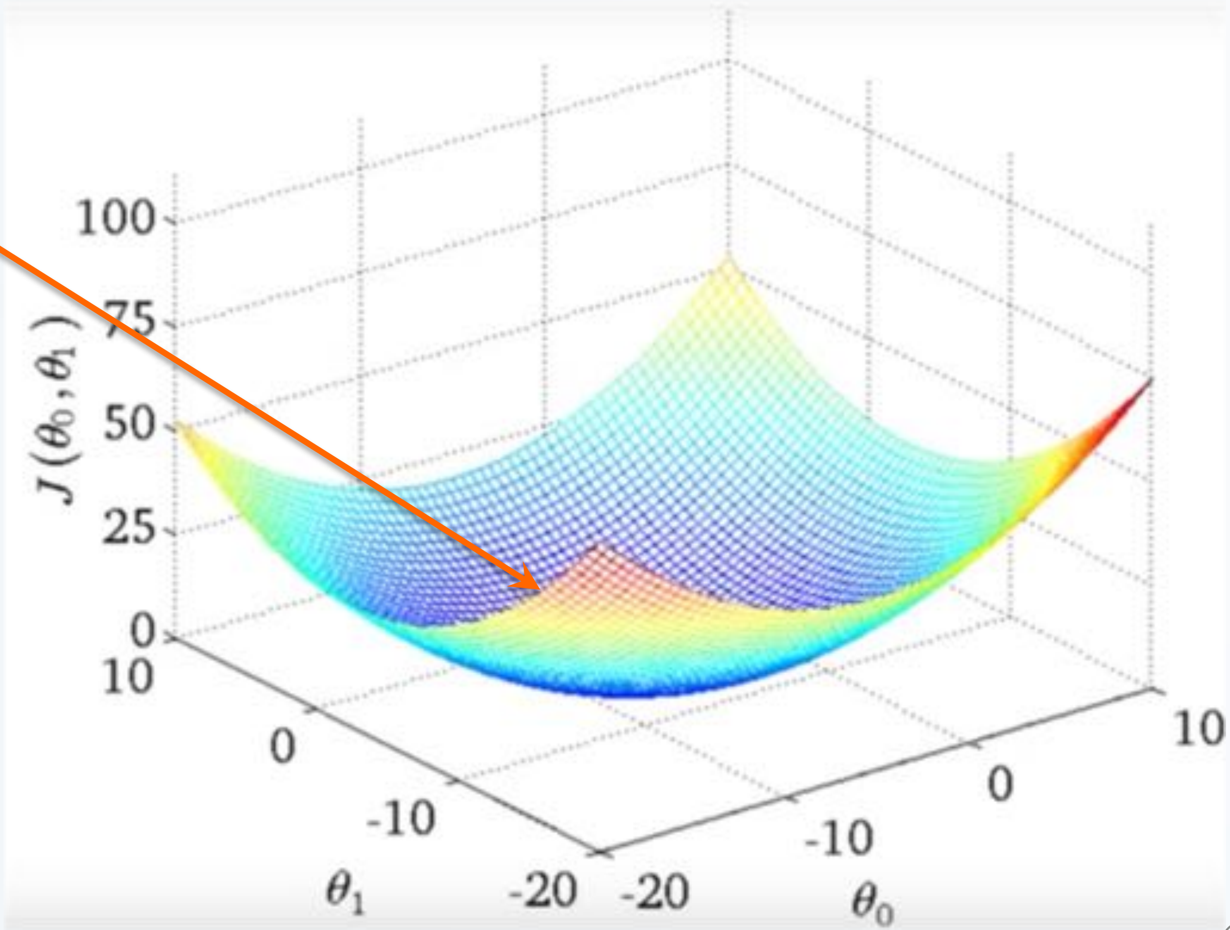
Cost Function: $J(\theta_0, \theta_1) = \dfrac{1}{2m} \sum_{i=1}^{m} (h(x^i) - y^i)^2$

Our Goal: $\text{minimize } J(\theta_0,\ \theta_1)$

Cost Function Intuition II

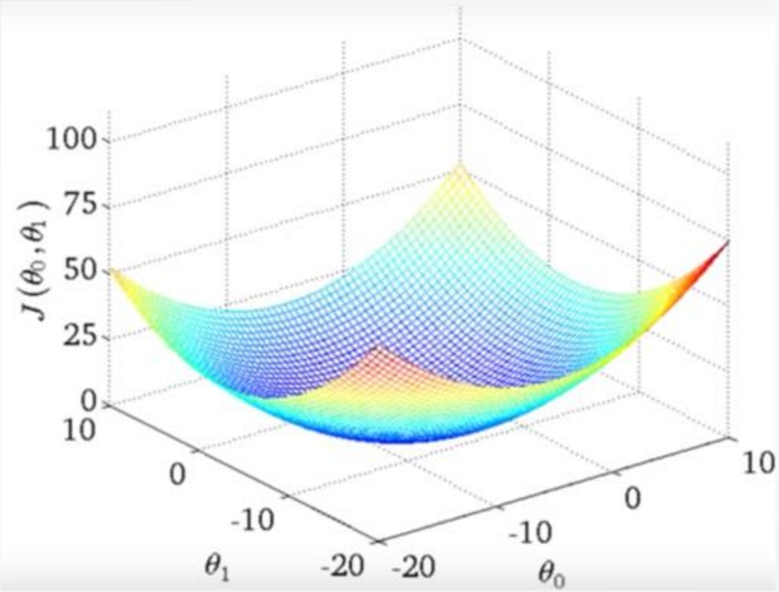
Given any dataset, when we try to draw the cost function $J(\theta_0, \theta_1)$, we may get this 3D shape:

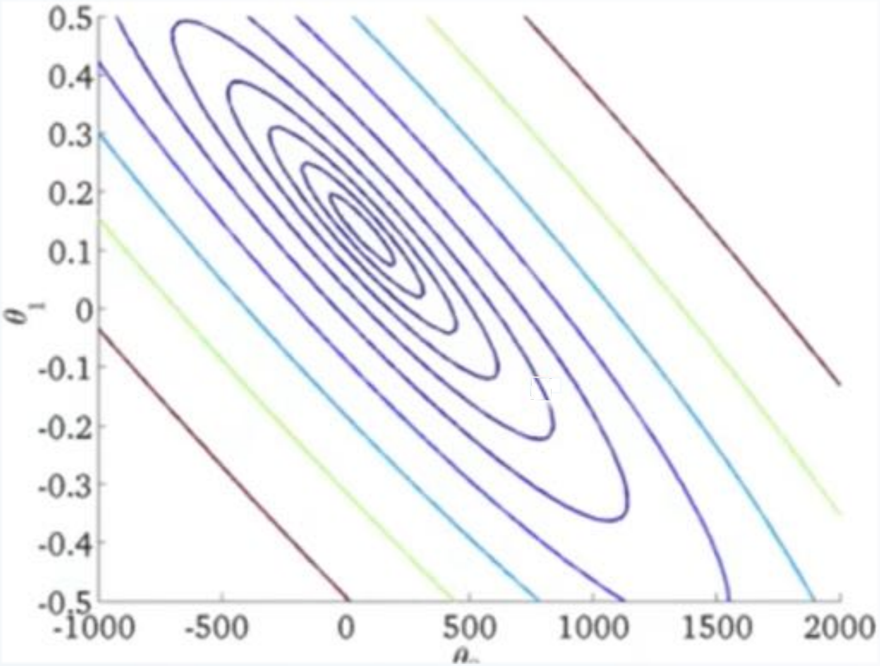
Given a dataset, our goal is find the minimum values of $J(\theta_0, \theta_1)$



Cost Function Intuition II

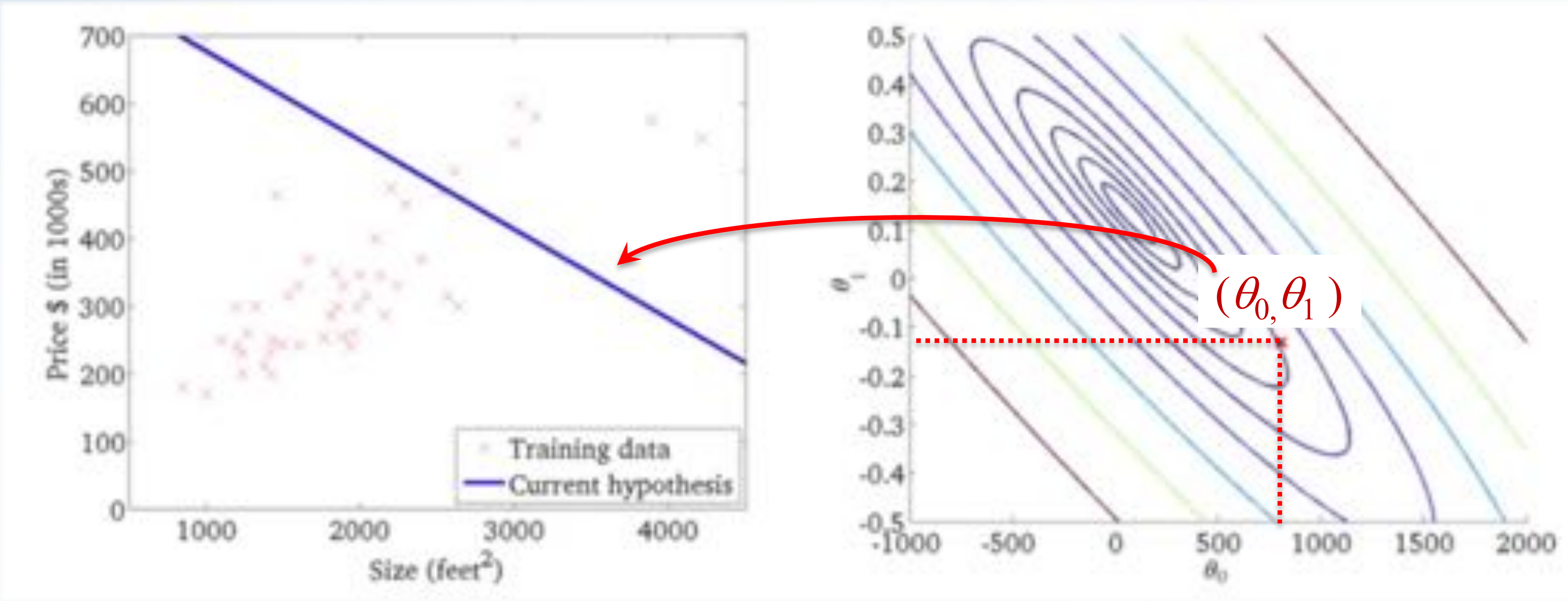
We may draw the cost function also using contour figures:





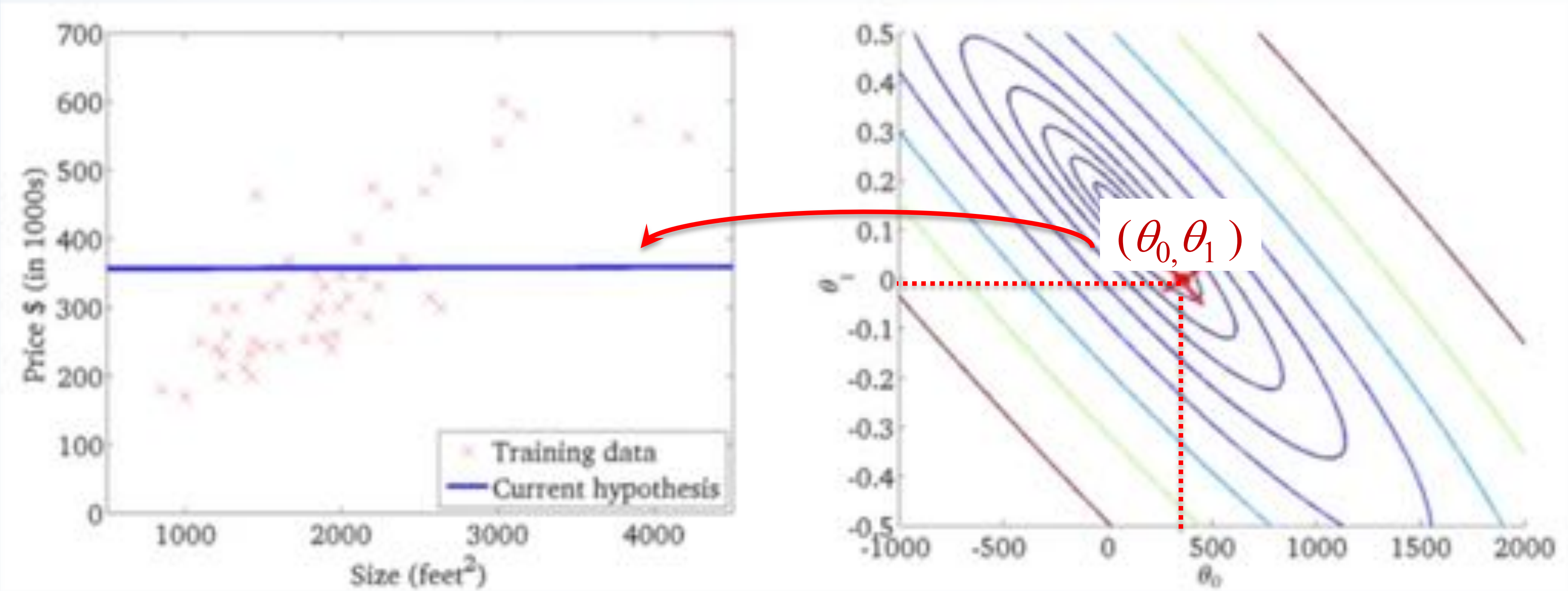
Cost Function Intuition II

$$h(x) = 800 + 0.15 \cdot x$$

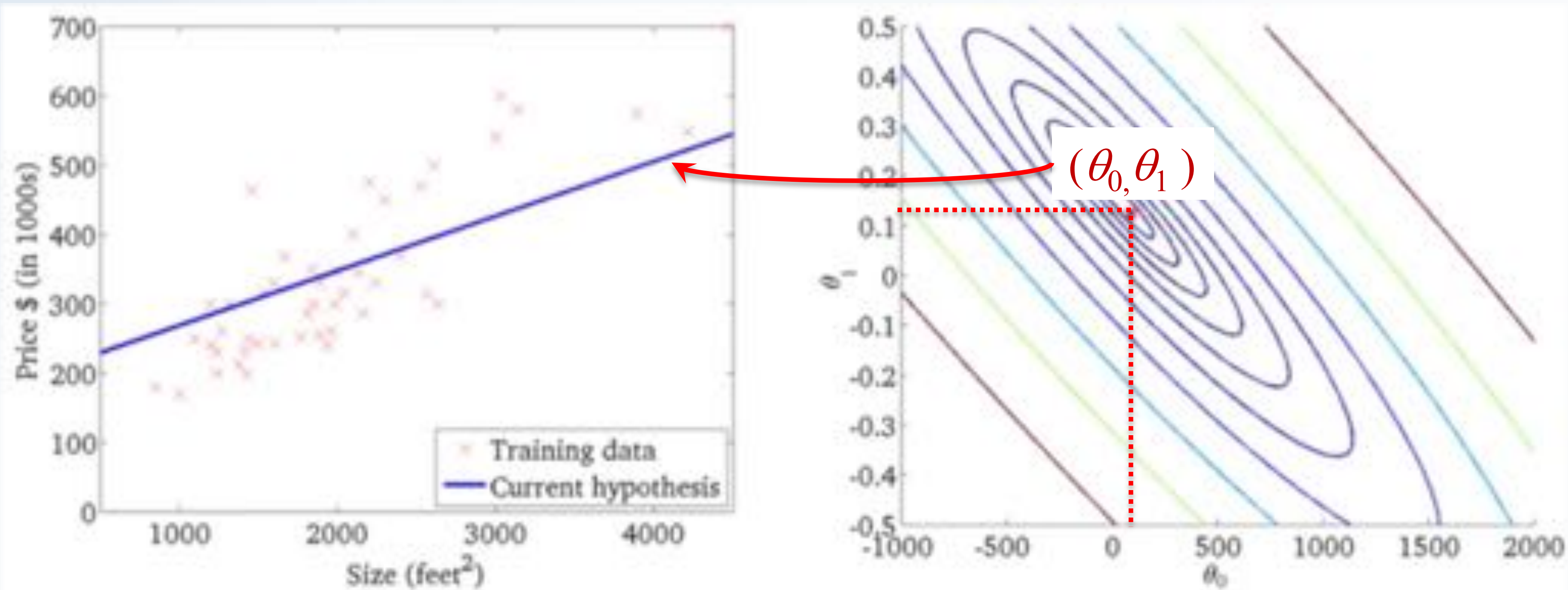


Cost Function Intuition II

$$h(x) = 360 + 0 \cdot x$$



Cost Function Intuition II



Is there any way/algorithm to find θs *automatically?*

Yes, e.g., the **Gradient Descent** Algorithm

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The **Gradient Descent** Algorithm

Starts with some initial values of θ_0 and θ_1

Keep changing θ_0 and θ_1 to reduce $J(\theta_0, \theta_1)$

Until hopefully we end up at a minimum

J is 0 or 1

Repeat until convergence {

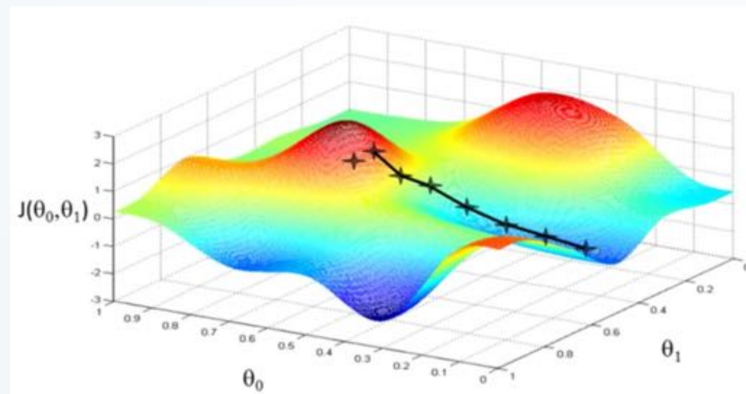
$$Temp0 := \theta_0 - \alpha \,.\, \frac{\partial}{\partial \theta_0} \,.\, J(\theta_0, \theta_1)$$

$$Temp1 := \theta 1 - \underbrace{\alpha}_{\text{Learning Rate}} \,.\, \underbrace{\frac{\partial}{\partial \theta_1} \,.\, J(\theta_0, \theta_1)}_{\text{Partial Derivation}}$$

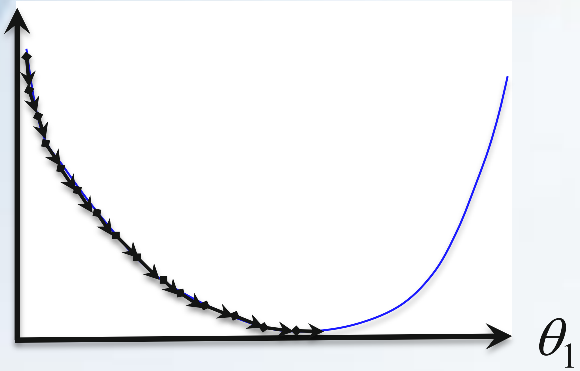
$$\theta_0 := Temp0$$

$$\theta_1 := Temp1$$

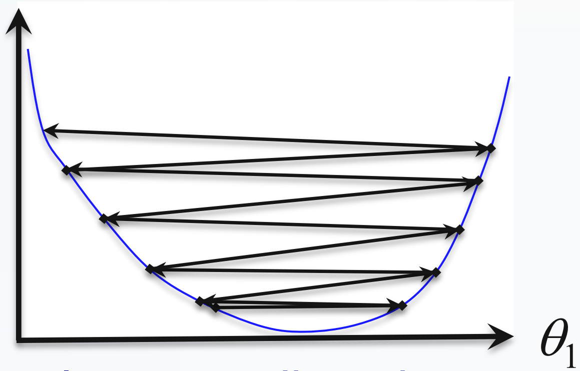
}



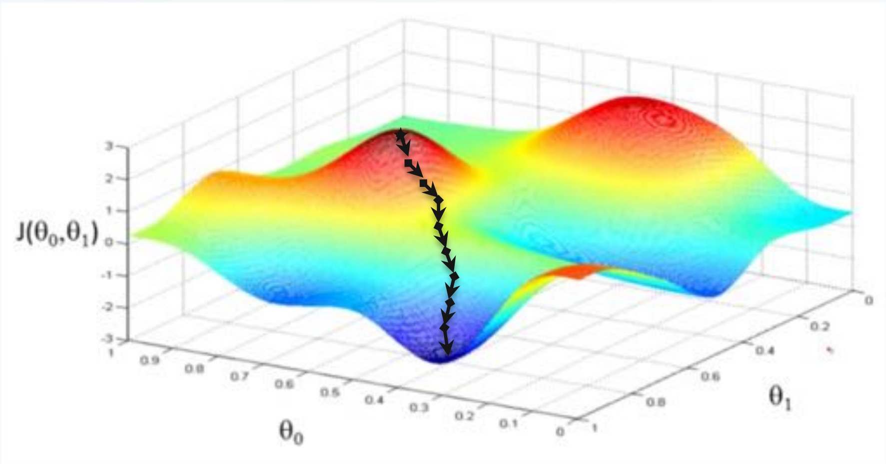
The Problem of the Gradient Descent algo.



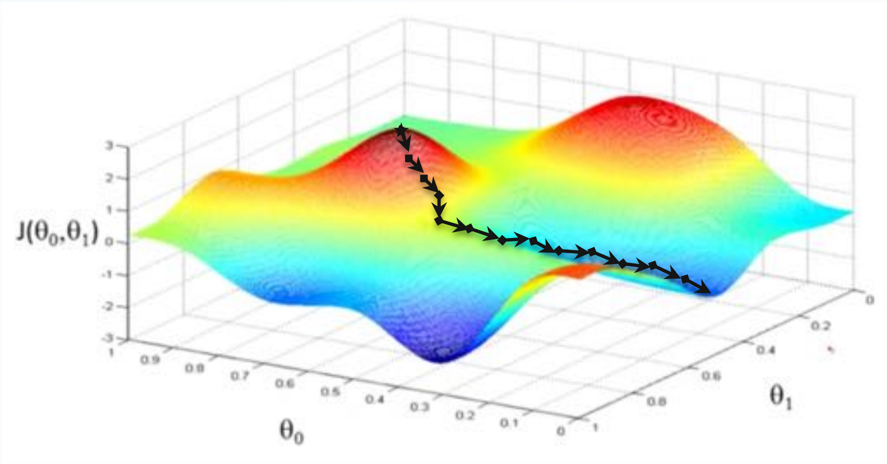
If α is too small, gradient descent can be slow



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



May converge to *global* minimum



May converge to a *local* minimum

The Gradient Descent for Linear Regression

Simplified version for linear regression

J is 0 and 1

Repeat until convergence {

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

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

}

Next, we will try to use Linear Algebra to *numerically* minimize θs (called **Normal Equation**) without needing to use iterating algorithms like Gradient Descent. However Gradient Descent scales better for bigger datasets.

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Minimizing θs numerically

Another way to numerically (using linear algebra) estimate the optimal values of θs.

Given the following features:

x_1 Size ft^2	x_2 bedrooms	x_3 floors	x_4 Age	y Price
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

Convert the features and the target value into matrixes:

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

Minimizing θs numerically

x_1 Size ft^2	x_2 bedrooms	x_3 floors	x_4 Age	y Price
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

add x_0, so to represent θ_0

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

The Normal Equation

To obtain the optimal values (minimized) of θs,
Use the following **Normal Equation**:

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

Where:

θ: the set of θs we want to minimize
X: the set of features in the training set
y: the output values we try to predict
X^T: the transpose of X
X^{-1}: the inverse of X

In Octave: `pinv(X'*X)*X' *y`

Gradient Descent Vs Normal Equation

m **training examples,** ***n*** **features**

Gradient Descent	**Normal Equation**
• Needs to choose the learning rate (α)	• No need to choose (α)
• Needs many iterations	• Don't need to iterate
• Works well even when n is large	• Need to compute (X^TX), which takes about $O(n^3)$
	• Slow if n is very large
	• Some matrices (e.g., singular) are non-invertible

Recommendation: use the Normal Equation If the number of features in less than 1000, otherwise the Gradient Descent.

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Matrix Vector Multiplication

$$\begin{bmatrix} 1 & 3 \\ 4 & 0 \\ 2 & 1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 5 \end{bmatrix} = \begin{bmatrix} 16 \\ 4 \\ 7 \end{bmatrix}$$

$$1 \times 1 + 3 \times 5 = 16$$

$$4 \times 1 + 0 \times 5 = 4$$

$$2 \times 1 + 1 \times 5 = 7$$

Matrix Matrix Multiplication

$$\begin{bmatrix} 1 & 3 & 2 \\ 4 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 3 \\ 0 & 1 \\ 5 & 2 \end{bmatrix} = \begin{bmatrix} 11 & 10 \\ 9 & 14 \end{bmatrix}$$

Multiple with the first column

$$\begin{bmatrix} 1 & 3 & 2 \\ 4 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 0 \\ 5 \end{bmatrix} = \begin{bmatrix} 11 \\ 9 \end{bmatrix}$$

Multiple with the second column

$$\begin{bmatrix} 1 & 3 & 2 \\ 4 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 10 \\ 14 \end{bmatrix}$$

Matrix Inverse

If A is an $m \times m$ matrix, and if it has an inverse, then

$$A \times A^{-1} = A^{-1} \times A = I$$

The multiplication of a matrix with its inverse produce an identity matrix:

$$\begin{bmatrix} 3 & 4 \\ 2 & 16 \end{bmatrix} \times \begin{bmatrix} 0.4 & -0.1 \\ -0.05 & 0.075 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Some matrices do not have inverses e.g., if all cells are zeros
For more, please review Linear Algebra

Matrix Transpose

Example: $A = \begin{bmatrix} 1 & 2 & 0 \\ 3 & 5 & 9 \end{bmatrix}$ $A^T = \begin{bmatrix} 1 & 3 \\ 2 & 5 \\ 0 & 9 \end{bmatrix}$

Let A be an $m \times n$ matrix, and let $B = A^T$
Then B is an $n \times m$ matix, and $B_{ij} = A_{ji}$

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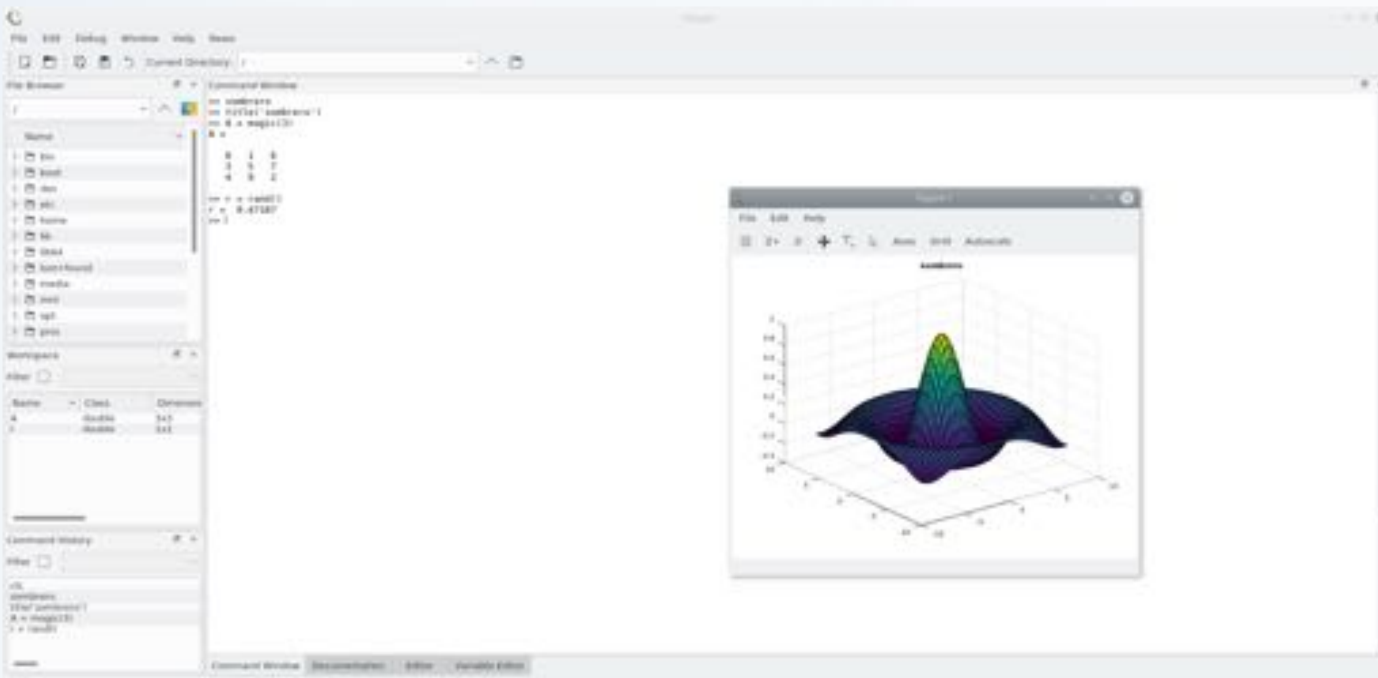
Octave

- Download from https://www.gnu.org/software/octave/
- High-level Scientific Programming Language
- Free alternatives to (and compatible with) Matlab
- helps in solving linear and nonlinear problems numerically



Online Tutorial https://www.youtube.com/playlist?list=PLnnr1O8OWc6aAjSc50lzzPVWgjzucZsSD

Compute the normal equation using Octave

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

In Octave:

```
load X.txt
load y.txt
C= pinv(X'*X)*X' *y
Save θ.txt
```

$\theta = \begin{bmatrix} 188.4 \\ 0.4 \\ -56 \\ -93 \\ -3.7 \end{bmatrix}$

These are the values of θs we need to use in our hypothesis function h(x)

$$h(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

$$h(x) = 188.4 + 0.4x - 56x^2 - 93x^3 - 3.7x^4$$

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R (programming language)

Free software environment for statistical computing and graphics that is supported by the R Foundation for Statistical Computing.

R comes with many functions that can do sophisticated stuff, and the ability to install additional packages to do much more.

Download R: https://cran.r-project.org/

A very good IDE for R is the RStudio:
https://www.rstudio.com/products/rstudio/download/

R basics tutorial:
https://www.youtube.com/playlist?list=PLjgj6kdf_snYBkIsWQYcYtUZiDpam7ygg

Compute the normal equation using R

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

In R:

```
X = as.matrix(read.table("~/x.txt", header=F, sep=","))
Y = as.matrix(read.table("~/y.txt", header=F, sep=","))

thetas = solve( t(X) %*% X ) %*% t(X) %*% Y

write.table(thetas, file="~/thetas.txt",
            row.names=F, col.names=F)
```

t(X): is the transpose of matrix X.
solve(X): is the inverse of matrix X.

References

[1] Andrew Ng's course about Machine Learning
https://www.youtube.com/channel/UCMoXOGX9mgrYNEwpcIQUcag

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[3] Mustafa Jarrar: Lecture Notes on Decision Tree Machine Learning, Birzeit University, 2018

[4] Mustafa Jarrar: Lecture Notes on Linear Regression Machine Learning, Birzeit University, 2018