

Regression



Overview

- Linear Regression Model
- Univariate Regression
- Gradient Descent & Normal Equation
- Multivariate Regression

Materials prepared based on PSU STAT414 (https://onlinecourses.science.psu.edu/stat414/print/book/export/html/262/) and machine learning by Andrew Ng.



Regression Model

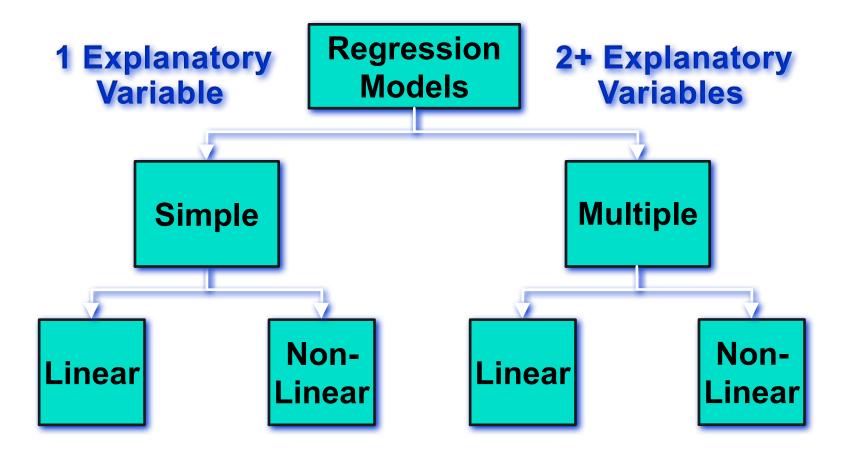
- Models are usually used for representation of some phenomenon
- Regression is a <u>predictive</u> modeling technique where the target to be estimated has a continuous variable type.

Examples:

- Predicting S&P 500 index using economic indicators
- Forecast the amount if precipitation in a region based on characteristics of jet stream
- Projecting the total sales of a company based on the amount of spending for advertisement



Types of Regression Models





Preliminaries

Let *D* denote a dataset of *N* observations $D = \{(\mathbf{x}_i, y_i) | i=1..N\}$

- Each explanatory variable x_i corresponds to the set of attributes of the i-th observation (x_i is also called predictor variable or independent variable)
- The corresponding target variable y_i is also called response variable, outcome variable or dependent variable.
- The explanatory variables of a regression can be either discrete or continuous.



Preliminaries

Predict housing price based on size, number of bed rooms, number of floors, and age of the house.

Size (feet ²)	Number of bedrooms	Number of floors	Age of home (years)	Price (\$1000)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

Explanatory variable Predictor variable Independent variable

Target variable Response variable Dependent variable



Regression

- Regression is the data mining task of <u>learning</u> a target function f that maps each attribute set
 x into a continuous-valued output y.
- The goal of regression is to find a target function that fits the input data with minimum error.
- Possible error functions:
 - Absolute Error = $\sum_{i} |y_{i} f(x_{i})|$
 - Squared Error = $\sum_{i} (y_i f(x_i))^2$



Simple Linear Regression

- Simple linear regression is a way of evaluating the relationship between two variables.
- For example, one might be interested in the relationship between:
 - heights and weights
 - high school grade point averages and college entrance exam scores
 - Housing price and size
 - speed and gas mileage
- Type of relationships
 - deterministic relationships
 - statistical relationships



Deterministic Relationships

- A deterministic (or functional) relationship is a hypothesized exact relationship between the predictor x and the response y.
- Example: the conversion between temperature in degrees Celsius (C) and degrees Fahrenheit (F)

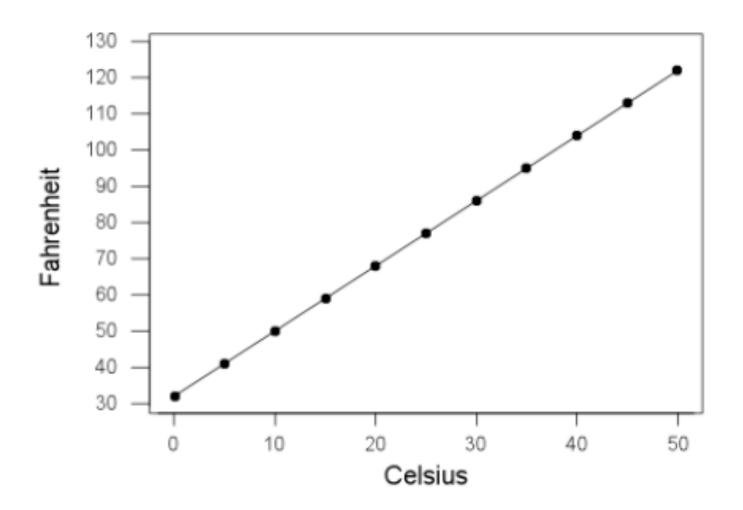
$$F=rac{9}{5}C+32$$

■ C=10

$$F = \frac{9}{5}(10) + 32 = 50$$



Celsius vs Fahrenheit





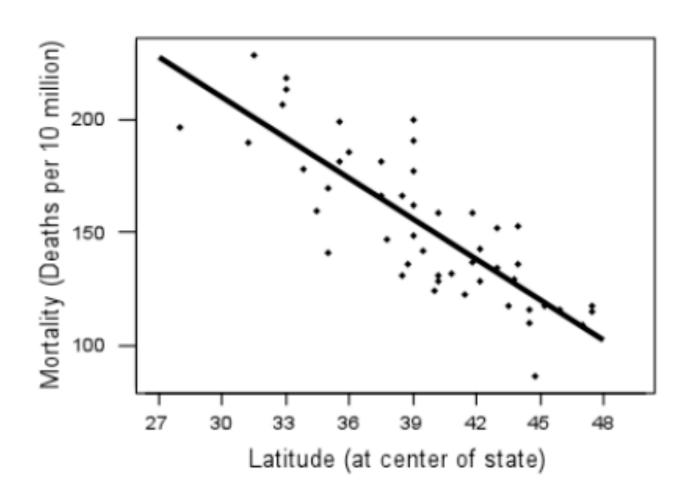
Statistical Relationship

- A statistical relationship is not an exact relationship.
- It is a scattered trend (less-than-perfect statistical relationships) existing between the predictor x and the response y.
- Example: relationship between the latitude (in degrees) at the center of each of the 50 U.S. states and the mortality (in deaths per 10 million) due to skin cancer in each of the 50 U.S. states
- Additional example: positive relationship between height and weight



Skin Cancer Mortality vs. State Latitude

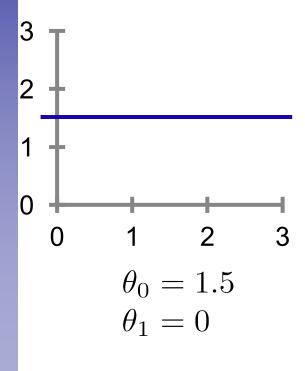
Skin cancer mortality versus State latitude

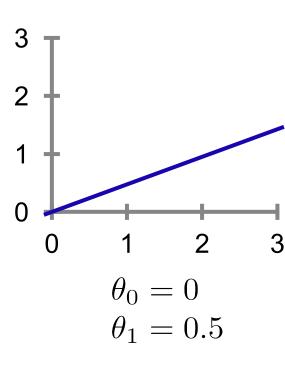


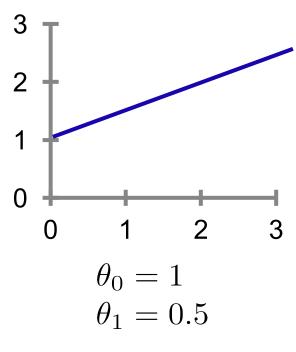
Linear Relationships

- Linear regression models model relationships by linear functions!
 - Use a linear function, i.e., line, to fit the observations.

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



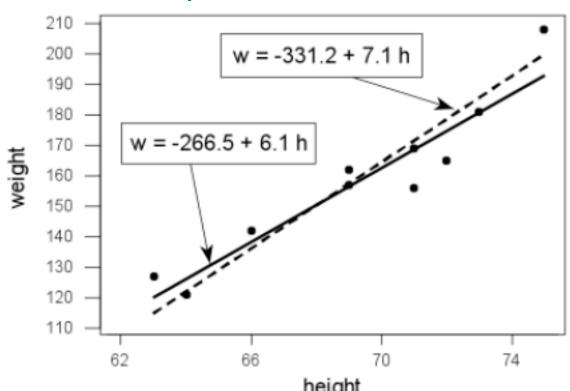






Least Squares: The Idea

- For example, to quantify an assumed linear relationship between height and weight
- Given ten observations, there are many fitting line.
 Summarize the relationship with the best fitting line, in terms of squared errors



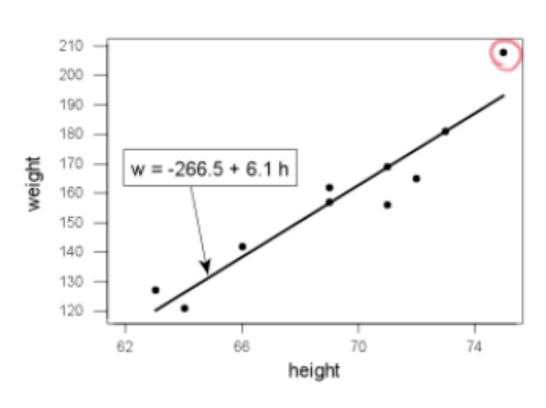


Finding Best Fitting Line

- Let y_i , x_i and $f(x_i)$ denote the observed response, the predictor value, and the predicted response (or fitted value) for the *i*-th observation.
- For the circled point
 - $x_i = 75 y_i = 208$
 - f(75) = -266.534 +6.13758(75) = 193.8
 - Prediction error:

$$e_i = y_i - f(x_i)$$

= 208-193.8
= 14.2





Least Squares Criterion

- A line that fits the data well will be one for which the n prediction errors are as small as possible.
- In order to find the best fitting line:

$$f(x_i) = a_1 + bx_i$$

We find a_1 and b that minimize the Sum of Squared prediction Errors:

$$SSE = \sum_{i=1..n} (y_i - f(x_i))^2 = \sum_{i=1..n} (y_i - (a_1 + bx_i))^2$$



Weight = $-331.2 + 7.1 \times Height$

i	$\mathbf{x_i}$	\mathbf{y}_{i}	$f(x_i)$	$y_i - f(x_i)$	$(y_i - f(x_i))^2$
1	64	121	123.2	-2.2	4.84
2	73	181	187.1	-6.1	37.21
3	71	156	172.9	-16.9	285.61
4	69	162	158.7	3.3	10.89
5	66	142	137.4	4.6	21.16
6	69	157	158.7	-1.7	2.89
7	75	208	201.3	6.7	44.89
8	71	169	172.9	-3.9	15.21
9	63	127	116.1	10.9	118.81
10	72	165	180.0	-15.0	225.00
					766.51



Weight = $-266.5 + 6.1 \times Height$

i	\mathbf{x}_{i}	y i	f(x _i)	y_i -f(x_i)	$(y_i - f(x_i))^2$
1	64	121	126.271	-5.3	28.09
2	73	181	181.509	-0.5	0.25
3	71	156	169.234	-13.2	174.24
4	69	162	156.959	5.0	25.00
5	66	142	138.546	3.5	12.25
6	69	157	156.959	0.0	0.00
7	75	208	193.784	14.2	201.64
8	71	169	169.234	-0.2	0.04
9	63	127	120.133	6.9	47.61
10	72	165	175.371	-10.4	108.16
					597.28



Least Squares Method

- Given $f(x) = a_1 + bx$, then $SSE = \sum_{i=1..n} (y_i - f(x_i))^2 = \sum_{i=1..n} (y_i - (a_1 + bx_i))^2$
- We minimize SSE to find a₁ and b
 - Statistical software, e.g., Minitab, can be used to find a₁
 and b
 - However, the intercept a1 (when x=0) is not very meaningful, e.g., let x and y be the height and weight.
 Then a₁ is the weight of a person with height = 0.
- Let $f(x) = a + b(x-\bar{x})$, where \bar{x} is the average of x values
 - The intercept *a* is the predicted weight of the person with average height.



Least Squares Estimate

The least squares regression line is:

$$f(x_i) = a + b(x_i - \bar{x})$$

with least squares estimates:

$$a=ar{y} \quad ext{ and } \quad b=rac{\sum\limits_{i=1}^n(x_i-ar{x})(y_i-ar{y})}{\sum\limits_{i=1}^n(x_i-ar{x})^2}$$

a is an estimate of intercept, and b is an estimate of the slope



Simple Linear Regression Model

- Consider the linear relationship between high school GPA x and scores on a college entrance exam Y, then x- \bar{x} is the centered GPA
- Assumption 1: Within the entire population of college students, there is a linear relationship between the average entrance score E(Y) and the centered GPA $x-\bar{x}$.

$$E(Y) = \alpha + \beta(x - \bar{x})$$

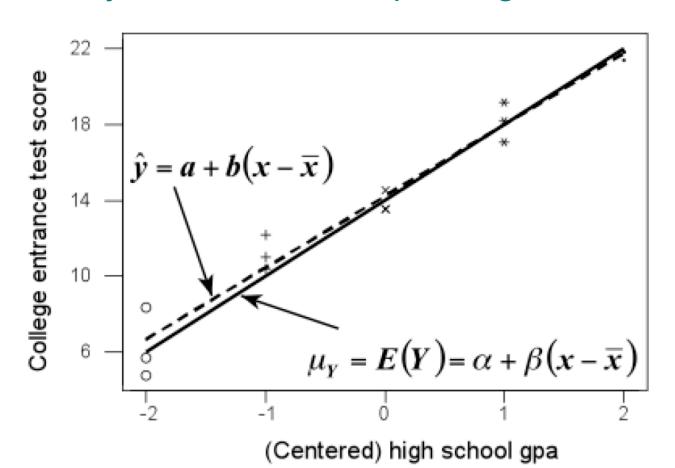
■ Assumption 2: individual students deviate from the mean entrance score of students with same centered GPA by some unknown amount ϵ_i .

$$Y_i = \alpha + \beta(x - \bar{x}) + \epsilon_i$$



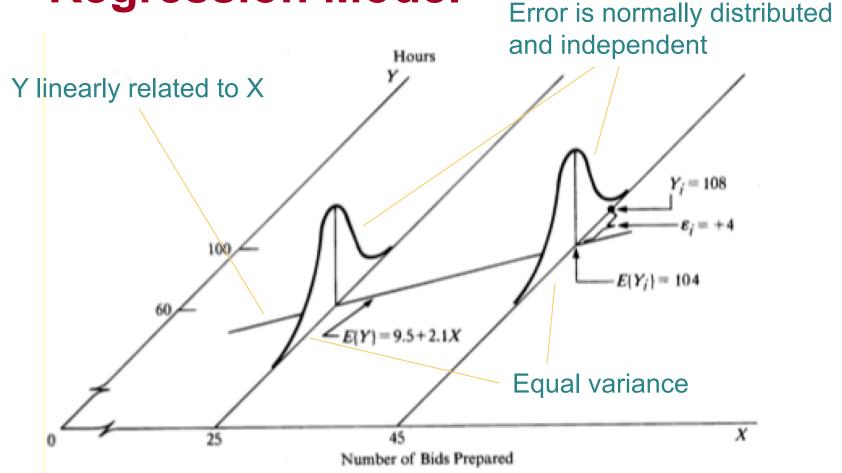
Simple Linear Regression Model

- As we do not have the data for the whole population, we cannot derive α and β .
- Best way is to estimae α , β using random samples.





Conditions for Simple Linear Regression Model





Simple Linear Regression Model

If the four conditions hold true, then:

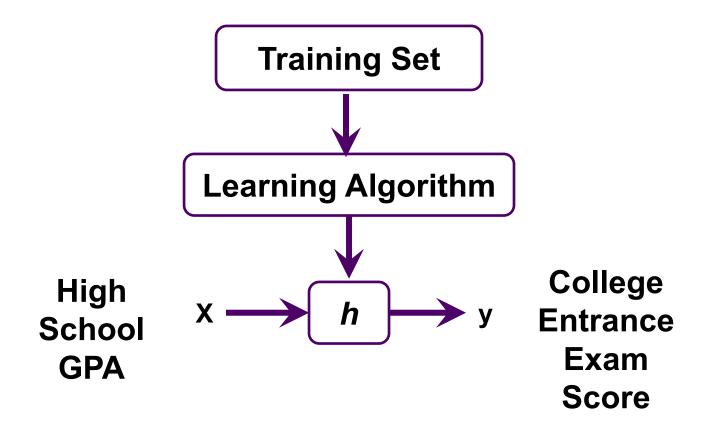
$$a=ar{y} \quad ext{ and } \quad b=rac{\sum\limits_{i=1}^n(x_i-ar{x})(y_i-ar{y})}{\sum\limits_{i=1}^n(x_i-ar{x})^2}$$

lacksquare a and b are the maximum likelihood estimators of α and β



Model Representation

Computer Science Point of View



How to learn/represent the model h as a good predictor of y?



Univariate Linear Regression

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

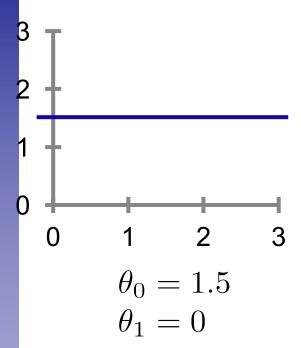
• Hypothesis:
$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

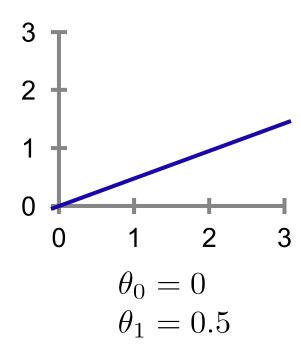
- Parameters: θ_i
- Regression Problem: How to choose θ_i such that $h_{\theta}(x)$ best fits the training set.

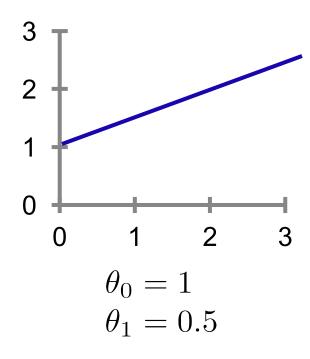


Linear Functions

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









Linear Regression Learning

■ Optimization problem: Choose θ (i.e., θ_0 , θ_1) so that h_θ is close to y in our training examples (x, y)

Hypothesis:

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

Parameters:

 θ_0, θ_1

(each represents one hypothesis function, i.e., one line.)

Objective (Cost) Function:

_ Average Squared Errors

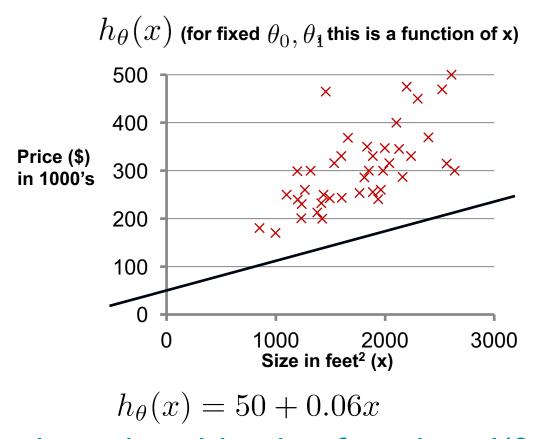
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$
 (function of θ_0 , θ_1)

Goal:
$$\min_{\theta_0,\theta_1} \text{ize } J(\theta_0,\theta_1)$$



Hypothesis vs. Objective (Cost)

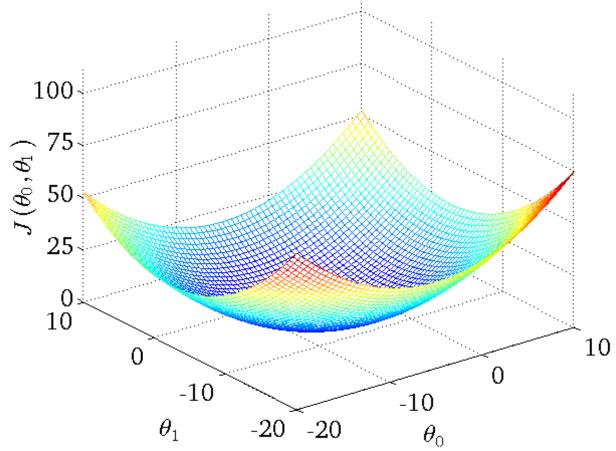
■ Plot of Hypothesis function $h_{\theta}(x)$



■ How does the objective function $J(\theta_0, \theta_1)$ look like graphically?



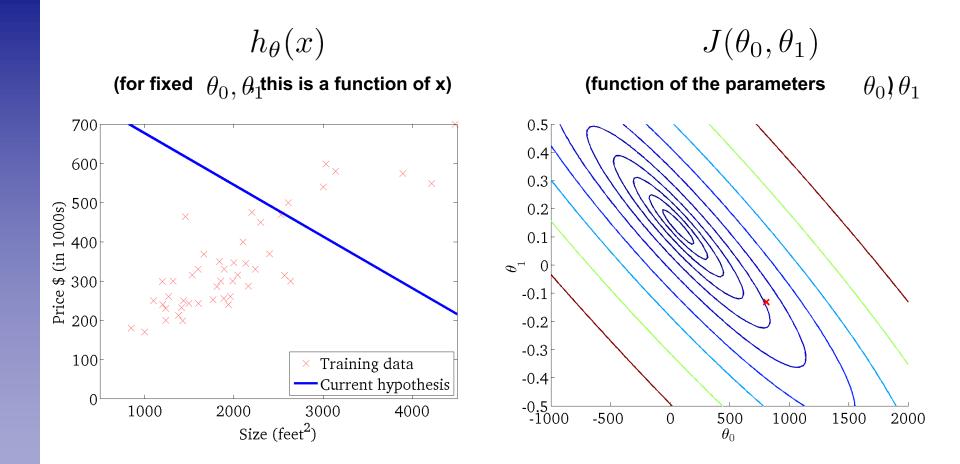
Graphical Plot of $J(\theta_0, \theta_1)$



■ Each θ (corresponding to a hypothesis function $h_{\theta}(x)$) is a point in the above figure of objective function $J(\theta_0, \theta_1)$

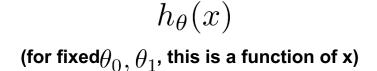


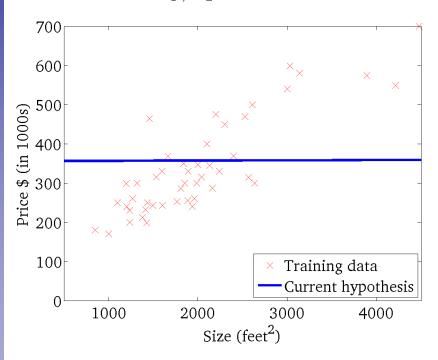
Contour Plot of $J(\theta_0, \theta_1)$



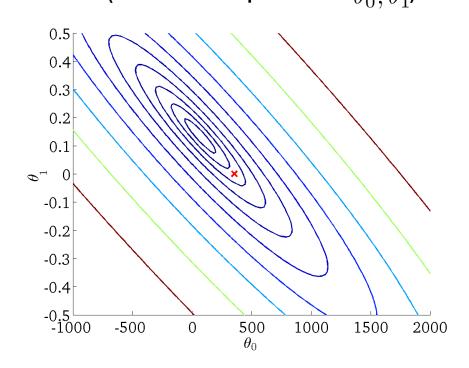


Contour Plot of $J(\theta_0, \theta_1)$



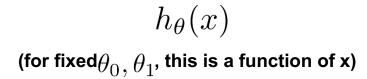


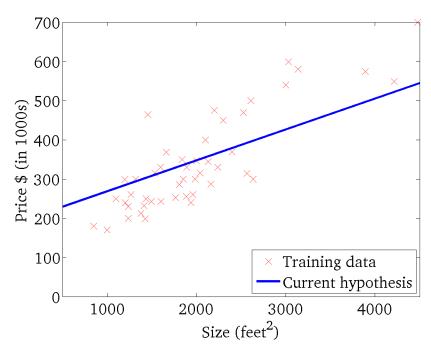
 $J(heta_0, heta_1)$ (function of the parameters $heta_0, heta_1$)



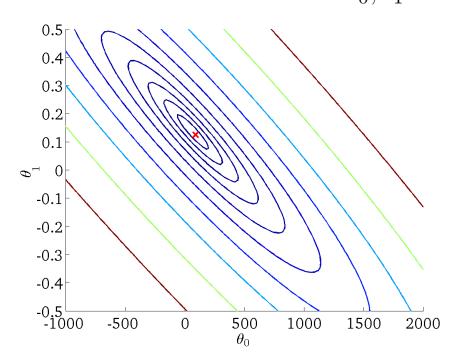


Contour Plot of $J(\theta_0, \theta_1)$





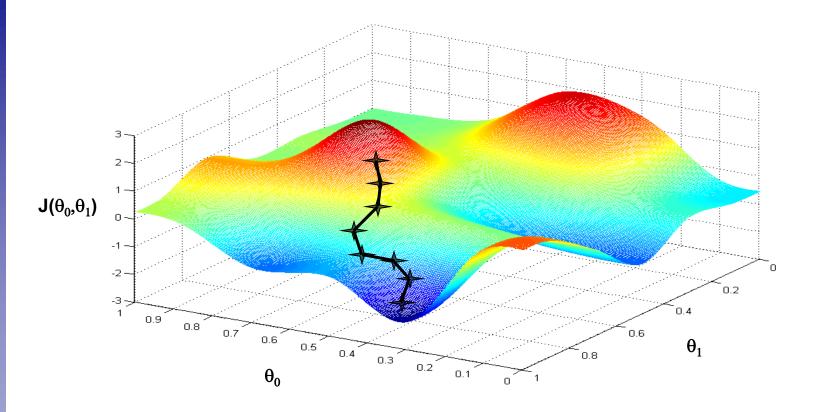
 $J(\theta_0,\theta_1)$ (function of the parameters θ_0,θ_1)

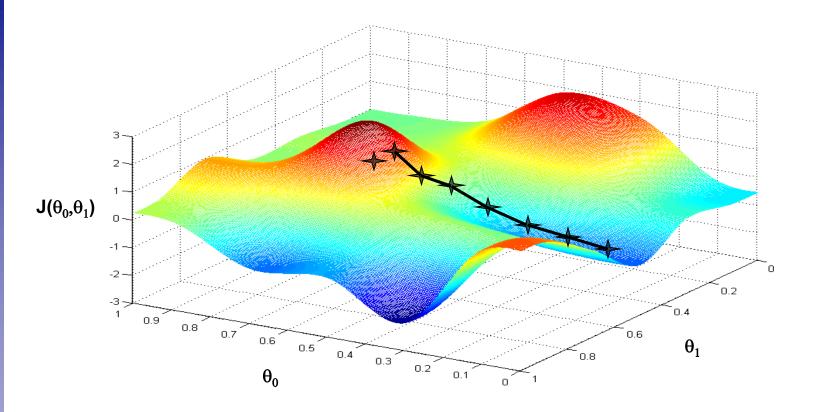




Gradient Descent

- Univariate Regression problem
 - Given: an objective function $J(\theta_0, \theta_1)$
 - Goal: $\underset{\theta_0,\theta_1}{\text{minimize}} J(\theta_0,\theta_1)$
- Idea:
 - 1. Start with some point (θ_0, θ_1)
 - 2. Iteratively updating (θ_0, θ_1) towards reducing $J(\theta_0, \theta_1)$ until reaching a minimum point
- Applicable for more general minimization problems, not only for regression problems.







Gradient Descent Algorithm

Repeat

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

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

- α is the learning rate, which determines the size of each step
- Update of parameters

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

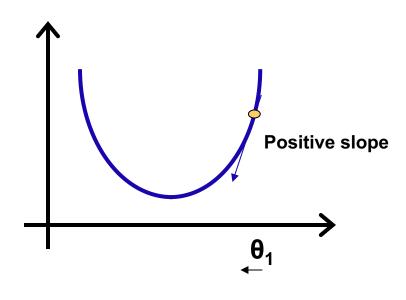
Incorrect (why?)

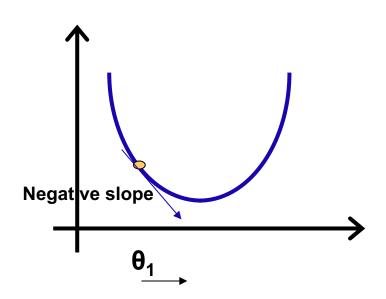


Gradient Descent: Intuition

■ Consider a simplified version of $J(\theta_1)$, i.e., θ_0 ,=0

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

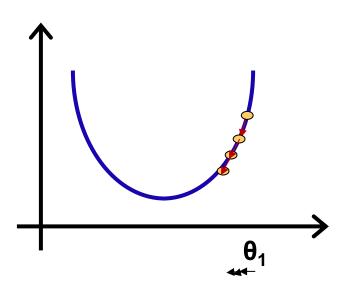


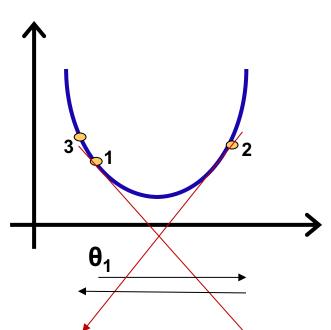




Effect of Learning Rate α

 \blacksquare Gradient descent can be very slow with a small α





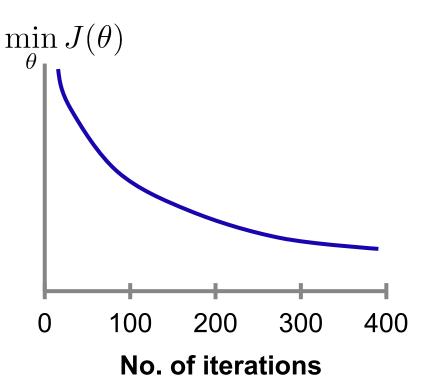
- With a large α , gradient descent can overshoot the minimum, and fail to converge, or even diverge.
- It's essential to find a proper learning date!

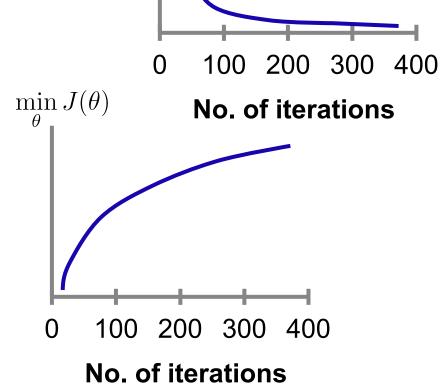


Setting of Learning Rate a

To make sure gradient descent working correctly, α needs to be set properly. $\min_{\min J(\theta)}$

■ As the no. of iterations increases, $J(\theta_1)$ is expected to decreased.

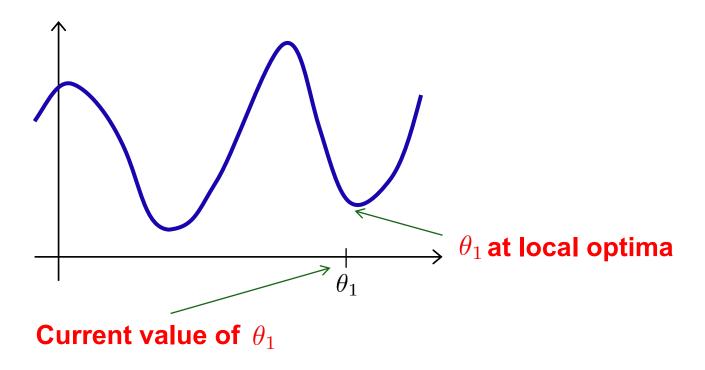






Local Minimum

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



 Gradient descent automatically takes smaller steps, when it approaches a local minimum,



Gradient Descent Algorithm for Linear Regression Model

Gradient Descent Algorithm

Repeat

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

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

Linear Regression Model

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



Gradient Descent Algorithm for Linear Regression Model

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

 Gradient Descent Algorithm for Linear Regression Repeat

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m \left(h_{\theta}(x^{(i)}) - y^{(i)} \right)$$
 (simultaneously update
$$j = 0 \text{ and } j = 1$$
)
$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m \left(h_{\theta}(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)}$$

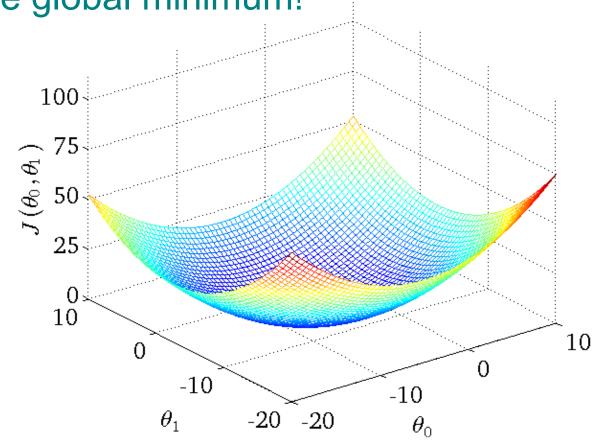
Until $J(\theta_0, \theta_1)$ converges

Each iteration involves all training samples

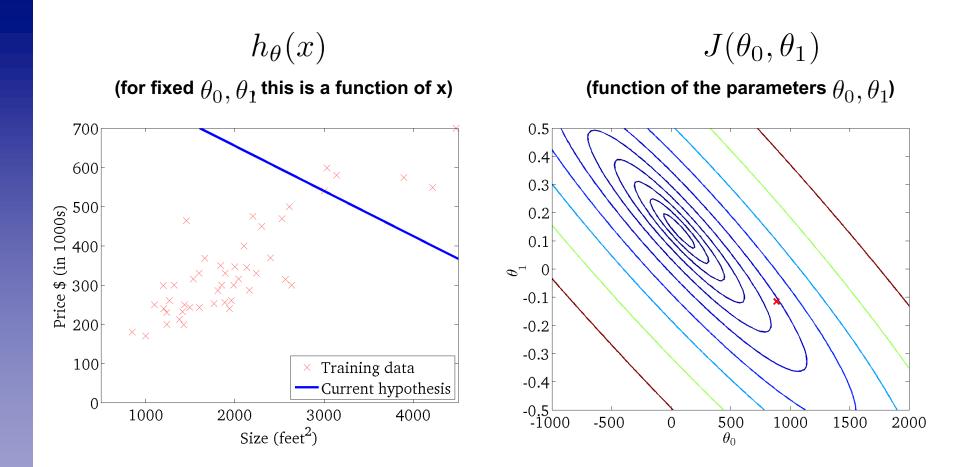


Convex Function

Objective function for Linear Regression is a bowl-shaped convex function, i.e., there is only one global minimum!

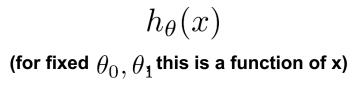


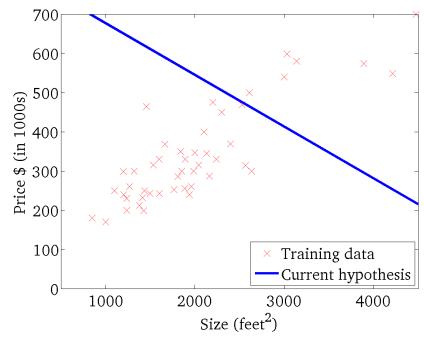




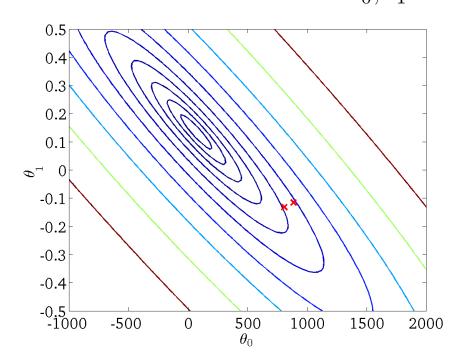
Initial point usually set at (0, 0) or randomly selected



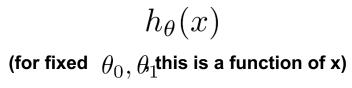


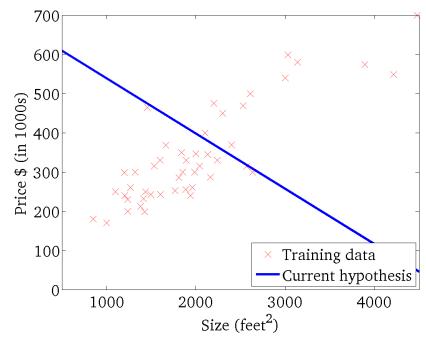


$J(\theta_0,\theta_1)$ (function of the parameters θ_0,θ_1)

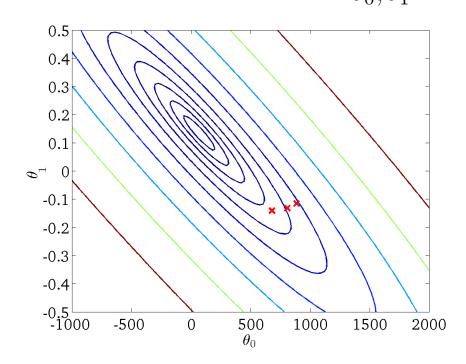




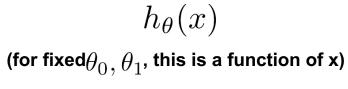


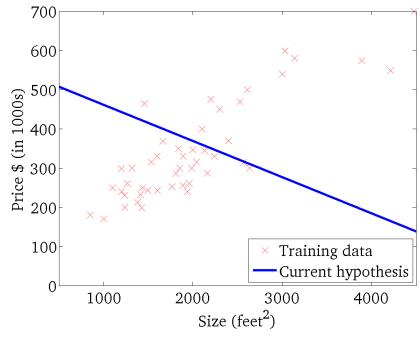


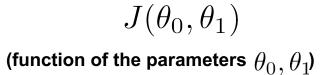
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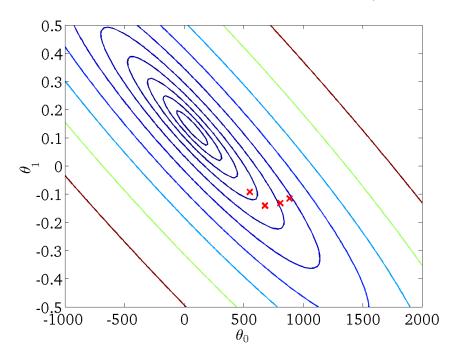




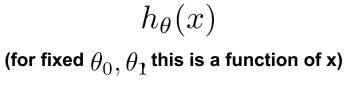


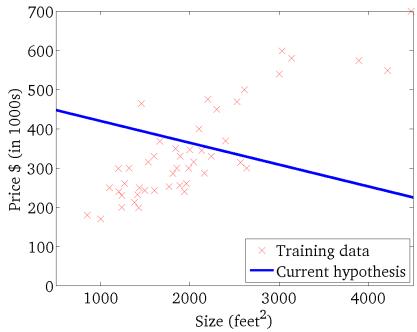




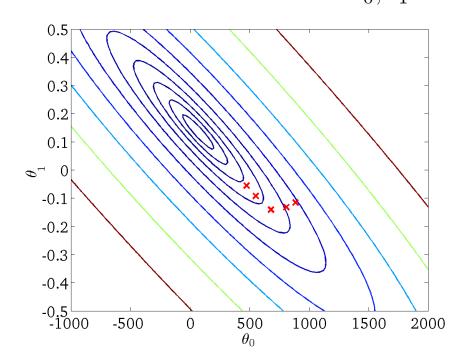




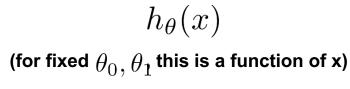


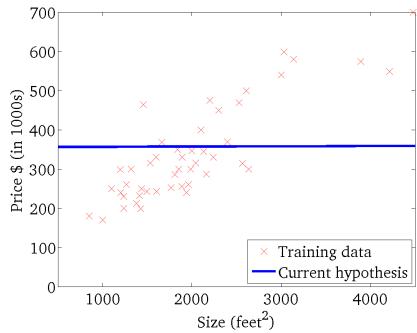


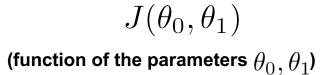
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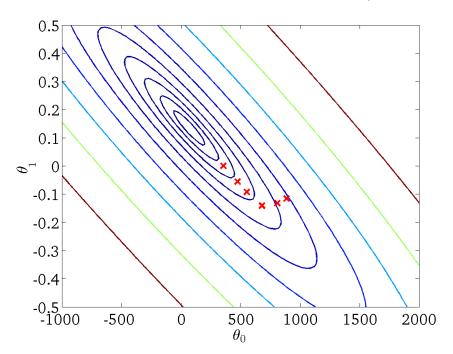




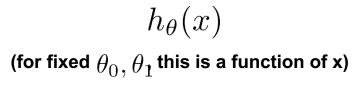


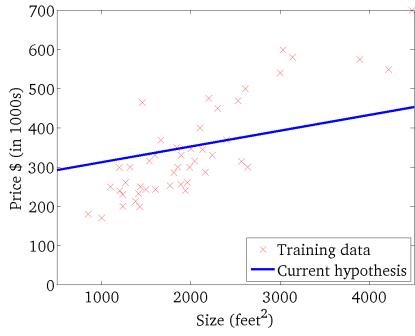




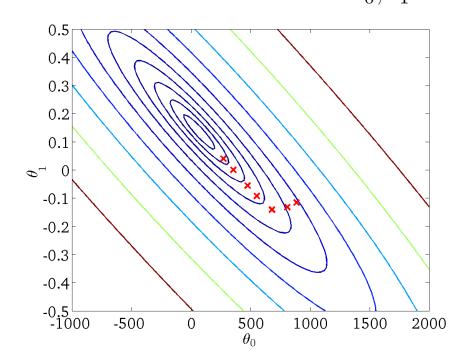




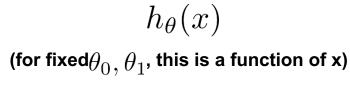


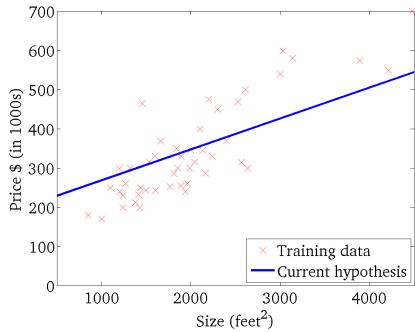


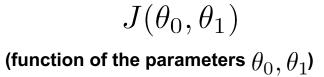
 $J(\theta_0,\theta_1)$ (function of the parameters θ_0,θ_1)

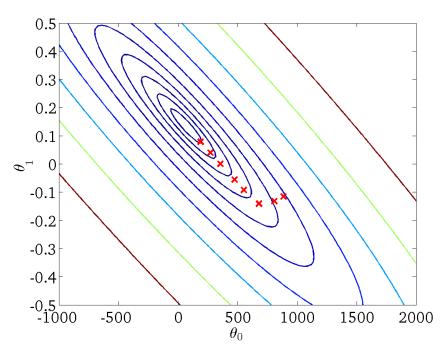




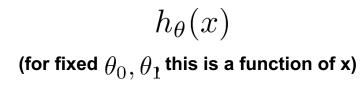


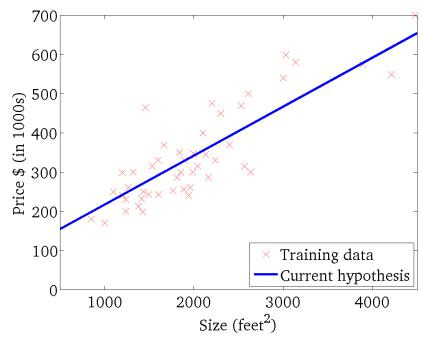


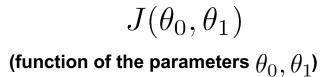


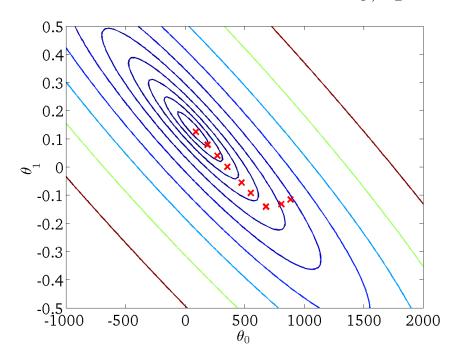














Alternative Approach

- Normal Equation: a numerical solution for solving linear regression equations without relying on the iterative approach of gradient descent.
- Gradient descent scales better than normal equation approach on large datasets



Normal Equation

■ Consider the objective function $J(\theta)$ for an

arbitrary θ .

• $J(\theta)$ is quadratic

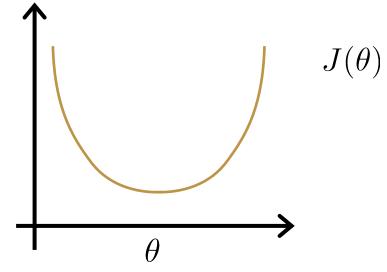
$$J(\theta) = a\theta^2 + b\theta + c$$

• To solve θ , we take

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

Solution:

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





Design Matrix: Univariate Regression

Predict housing price by size of the house

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

Design Matrix: X

$$X = \begin{bmatrix} 1 & 2104 \\ 1 & 1416 \\ 1 & 1534 \\ 1 & 852 \end{bmatrix} \qquad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$



Gradient Descent vs Normal Eq.

- Gradient descent (GD) is a iterative approach, while normal equation (NE) is numerical.
- GD needs to set a proper learning rate α but GD does not.
- GD needs perform normalization; NE does not
- GD works well even when the dataset is very large, but NE does not work that well.
 - NE needs to compute $(X^TX)^{-1}$ which is expensive when data size is large
 - $O(kn^2)$ vs $O(n^3)$ where n is the size of dataset



Multivariate Linear Regression

Multiple features

	Size (feet ²)	Number of bedrooms	Number of floors	Age of home (years)	Price (\$1000)
-	2104	5	1	45	460
(0)	1416	3	2	40	232
$\mathbf{X}^{(3)}$	1534	3	2	30	315
	852	2	1	36	178
		V			
		y			

Notation:

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



Hypothesis function

- x_0 =1 for convenience of notation
- $x = [x_0 \ x_1 \ x_2 \dots x_n]^T = [1 \ x_1 \ x_2 \dots x_n]^T$
- \bullet $\theta = [\theta_0 \ \theta_1 \ \theta_2 \ \dots \ \theta_n]^T$

$$h_{\theta}(x) = \begin{bmatrix} \theta_0 & \theta_1 & \dots & \theta_n \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} = \theta^T x$$



Multivariate Linear Regression Learning

■ Optimization problem: Choose θ (θ_0 , $\theta_{1, ...}$, θ_n) so that h_θ is close to y in our training examples (x, y)

Hypothesis:

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

Parameters:

$$\theta = \theta_0, \theta_1, \dots, \theta_n$$

Objective (Cost) Function:

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

Goal: minimize $J(\theta)$



Gradient Descent for Multivariate Linear Regression

Repeat

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

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

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



Data Preprocessing

Different scales of features/attributes Consider the housing dataset:

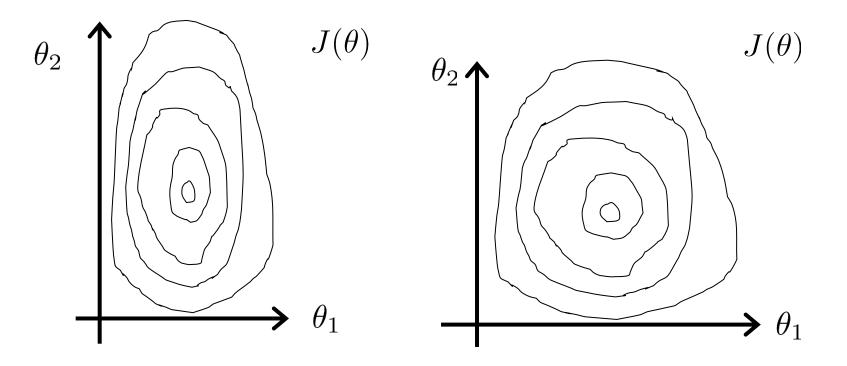
Size (feet²)	Number of bedrooms		Age of home (years)	Price (\$1000)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

■ The regression coefficients $\theta_{1,}$ $\theta_{2,...}$ and so on corresponding to features of different scales are expected to have different value ranges



Feature Normalization

- Gradient descent may be slowed down significantly.
- Descent slower in dimension of larger scale range



Normalization may bring scales into similar scale.



Feature Scaling

- Get every feature into approximately a [-1,1] range.
- Feature scaling divides the feature values by the range (i.e. the maximum value minus the minimum value) of the input variable.
- For example,
 - $x_1 = size (0-2000 feet^2)$ $\rightarrow x_1 = size /2000$
 - x_2 = number of bedrooms (1-5)
 - \rightarrow x_2 = number of bedroom/5



Mean Normalization

- Get every feature into approximately a [-0.5,0.5] range.
- Mean Normalization replaces the feature value x with $(x- \mu)$ divided the range (i.e. the maximum value minus the minimum value) of the input variable, where μ is the average feature value.
- Resulted features have approximately zero mean.
- For example,
 - $x_1 = size (0-2000 feet^2) \rightarrow x_1 = (size-1000) /2000$
 - x_2 = number of bedrooms (1-5)
 - $\rightarrow x_2 = (number of bedroom-2)/5$



Polynomial Regression

- Housing prices prediction
 - $h_{\theta}(x) = \theta_0 + \theta_1 Width + \theta_2 Depth$
- **■** Feature creation:
 - Area = Width * Depth
 - $h_{\theta}(x) = \theta_0 + \theta_1 Area$
- Depends on domain knowledge of the application
 - $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$ (Quadratic)
 - $h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$ (Cubic)
 - $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$ (Linear) where $x_1 = size$ $x_2 = size^2$ $x_3 = size^3$
- The tricks of linear regression can be applied to handle polynomial regression



Normal Equation (General Case)

■ Objective function J(θ) $\theta \in \mathbb{R}^{n+1}$

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

• To solve θ , for every j we take

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

Solution:

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

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Design Matrix: Multivariate Regression

		Size (feet²)	Number of bedrooms	Number of floors	Age of home (years)	Price (\$1000)
_	x_0	x_1	x_2	x_3	x_4	y
	1	2104	5	1	45	460
	1	1416	3	2	40	232
	1	1534	3	2	30	315
	1	852	2	1	36	178
	1	3000	4	1	38	540

Design Matrix X

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \\ 1 & 3000 & 4 & 1 & 38 \end{bmatrix} \quad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \\ 540 \end{bmatrix}$$