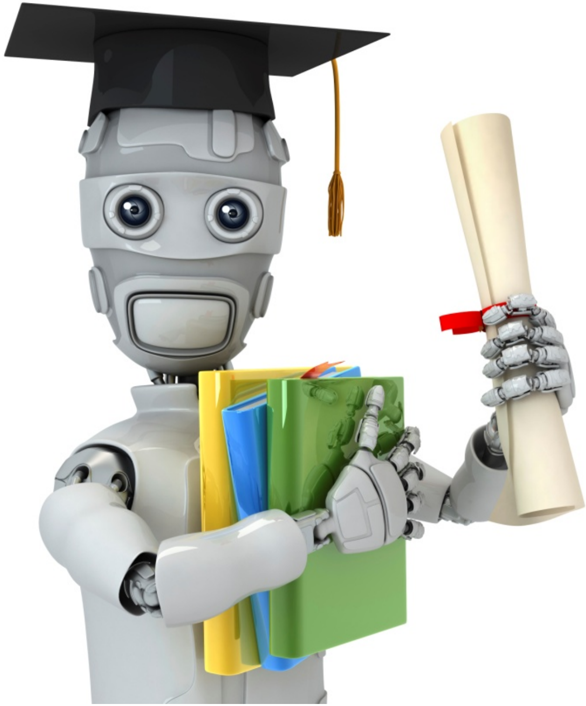

Machine Learning

Linear Regression with multiple variables

Multiple features

Multiple features (variables).

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

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

Multiple features (variables).

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

$m = 47$

Notation:

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

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

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

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Hypothesis:

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

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

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

age

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

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

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

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

$(n+1) \times 1$ matrix

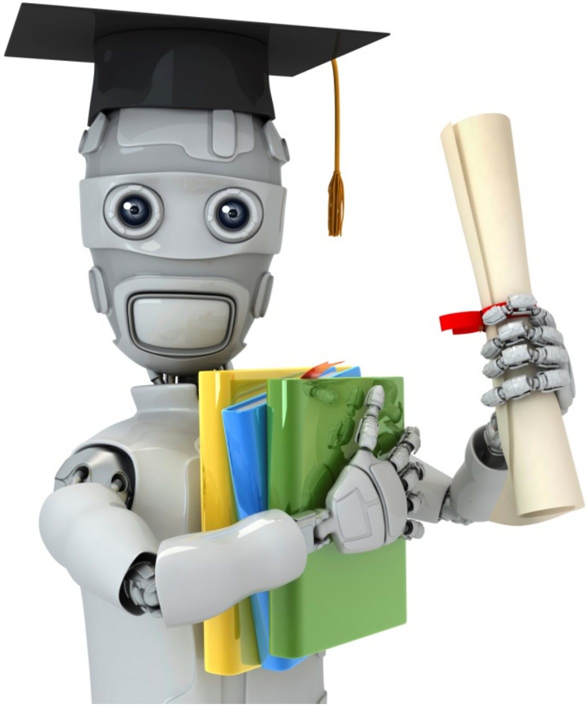
x

$\theta^T x$

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

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

Multivariate linear regression.



Machine Learning

Linear Regression with multiple variables

Gradient descent for multiple variables

$\longrightarrow x_0 = 1$

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

Cost function:

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

$J(\theta)$

Gradient descent:

Repeat $\{$

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

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

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Gradient Descent

Previously (n=1):

Repeat $\{$

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

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

$x^{(i)}$

(simultaneously update θ_0, θ_1)

$\}$

New algorithm $(n \geq 1)$:

Repeat $\{$

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

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

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

$\}$

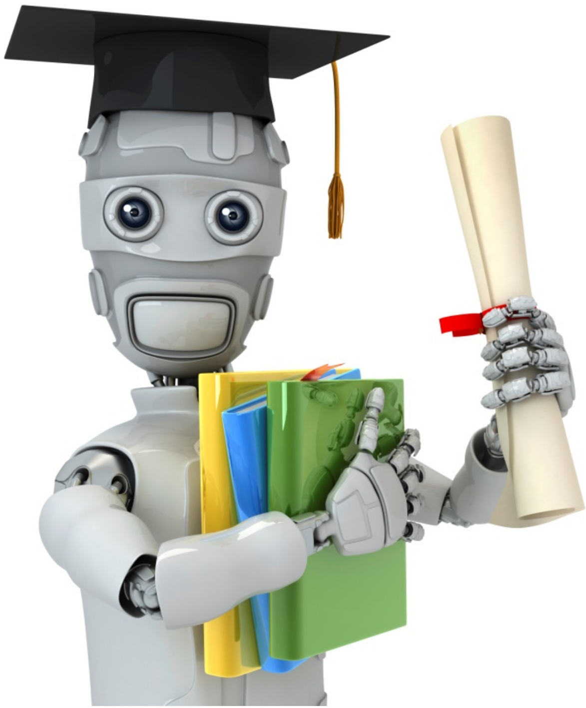
$x_0^{(i)} = 1$

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

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

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

$\ldots$



Machine Learning

Linear Regression with multiple variables

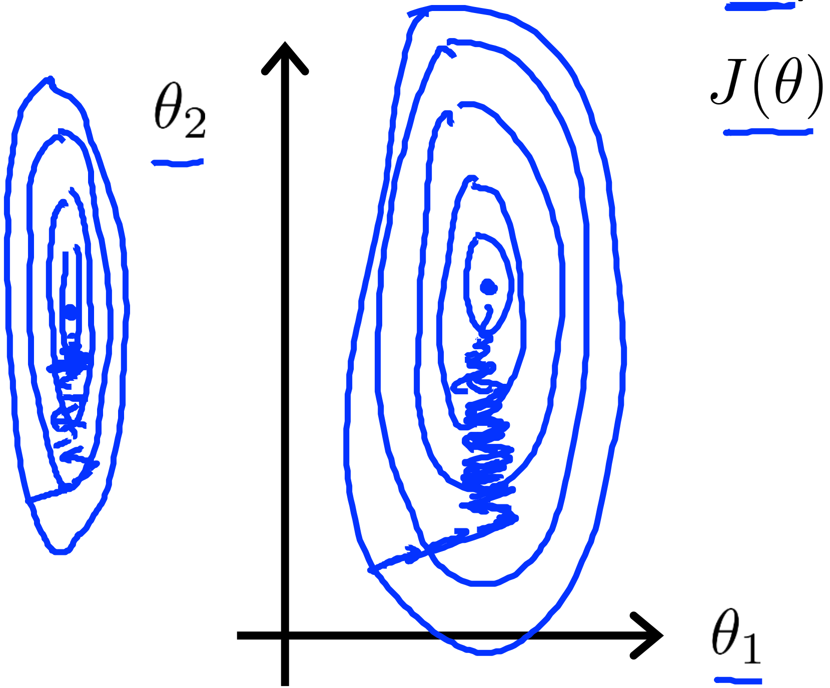
Gradient descent in practice I: Feature Scaling

Feature Scaling

Idea: Make sure features are on a similar scale.

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

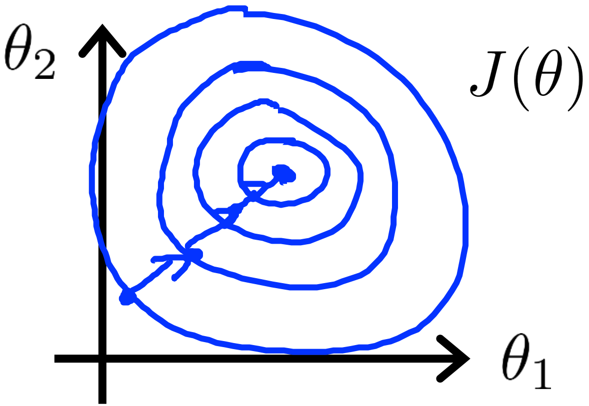
x_2 = number of bedrooms (1-5)



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

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

$0 \leq x_1 \leq 1 \qquad 0 \leq x_2 \leq 1$



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Feature Scaling

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

$x_0 = 1$

$0 \leq x_1 \leq 3$ ✓

$-2 \leq x_2 \leq 0.5$ ✓

$-100 \leq x_3 \boxed{100}$ ✗

$-0.0001 \leq x_4 \leq \boxed{0.0001}$ ✗

-3 to 3 ✓

$-\frac{1}{3}$ to $\frac{1}{3}$ ✓

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

Average size = 100

$\boxed{x_2 = \frac{\#bedrooms - 2}{5}}$ 4

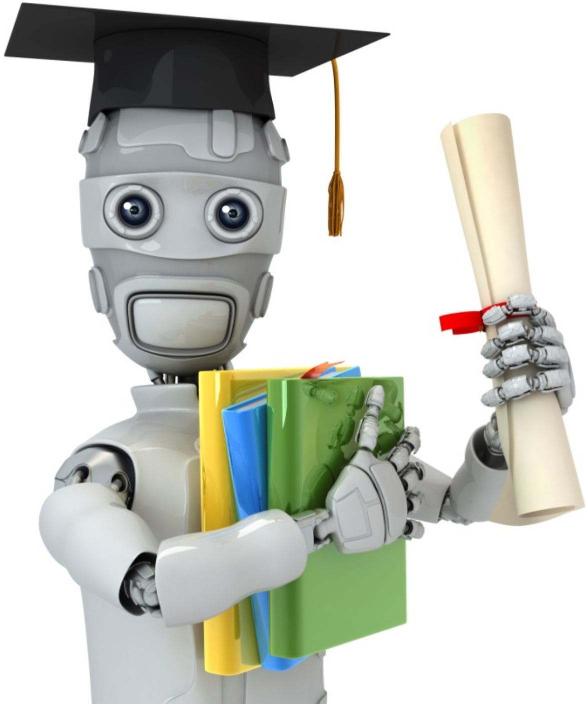
1-5 bedrooms

$\boxed{-0.5 \le x_1 \le 0.5}$, $\boxed{-0.5 \le x_2 \le 0.5}$

$x_1 \leftarrow \frac{x_1 - \mu_1}{s_1}$ ← avg value of x_1 in training set

s_1: range (max - min) (or standard deviation)

$x_2 \leftarrow \frac{x_2 - \mu_1}{s_2}$



Machine Learning

Linear Regression with multiple variables

Gradient descent in practice II: Learning rate

Gradient descent

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

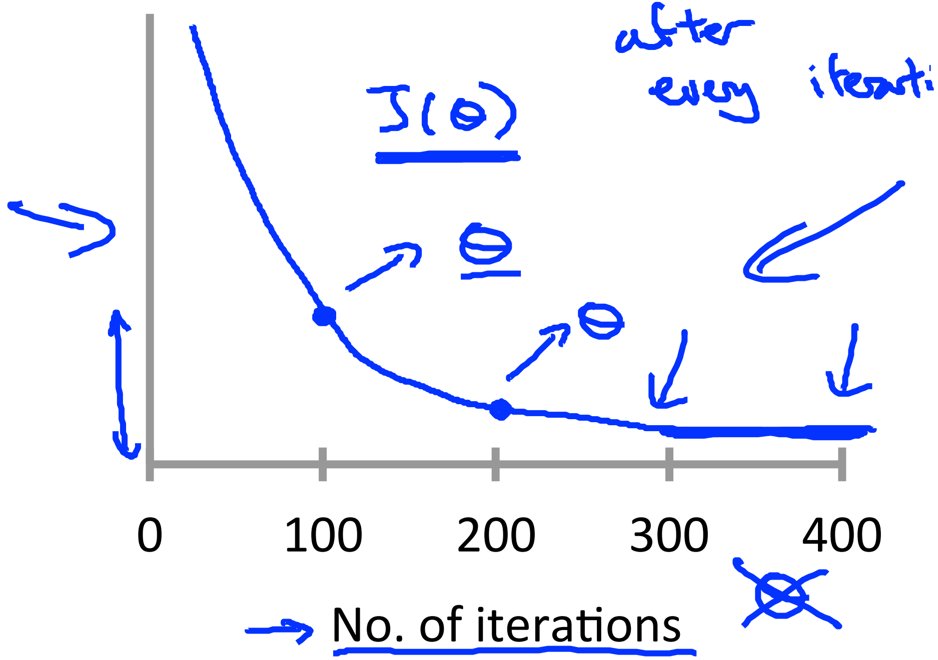
- "Debugging": How to make sure gradient descent is working correctly.

- How to choose learning rate $\boxed{\alpha.}$

Making sure gradient descent is working correctly.

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

J(θ) should decrease after every iteration



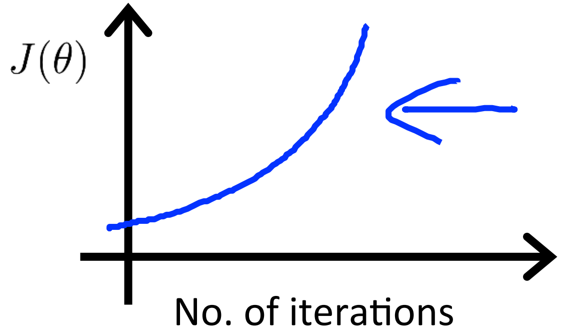
30, 3000, 3,000,000

→ Example automatic convergence test:

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

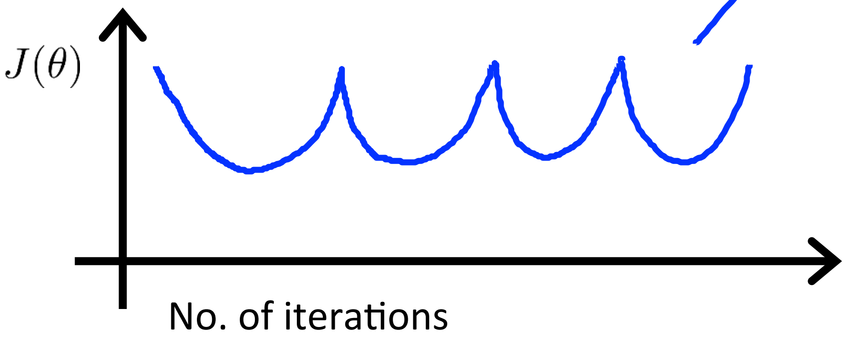
ε

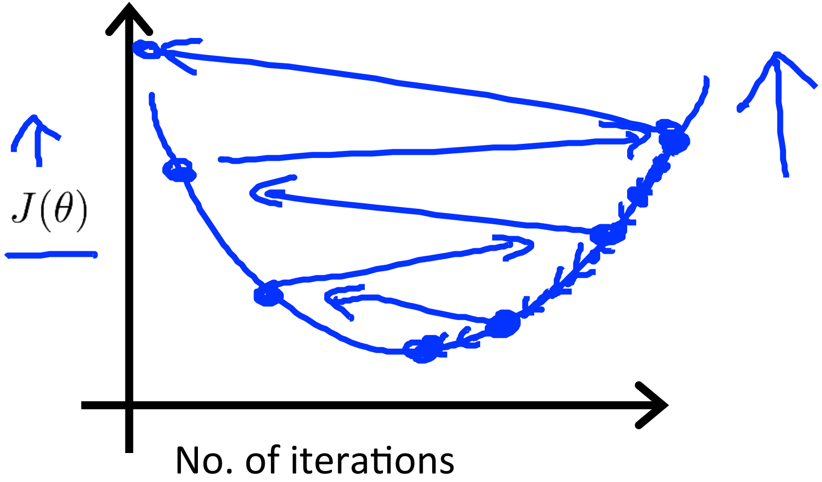
Making sure gradient descent is working correctly.



Gradient descent not working.

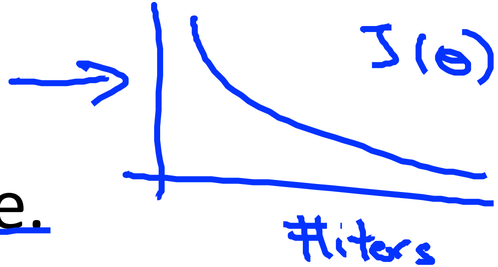
Use smaller α.





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

Summary:

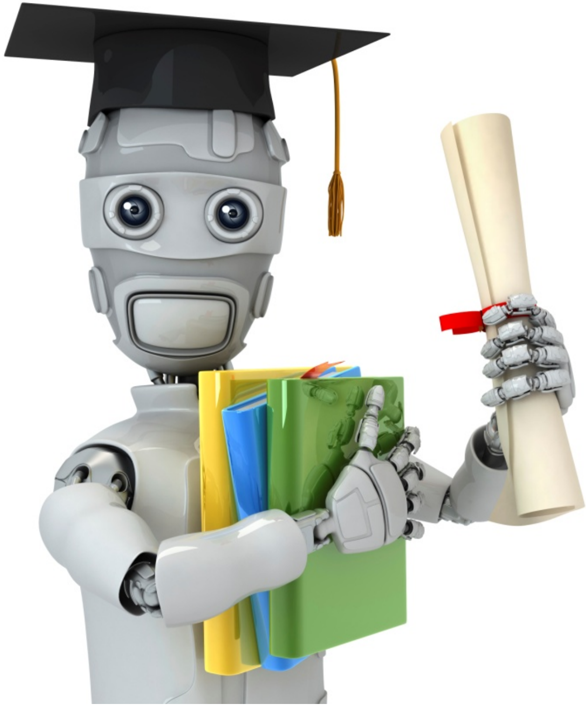


- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge. (Slow converge also possible)

To choose α, try

$$\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \ldots$$

3x ≈3x 3x ≈3x



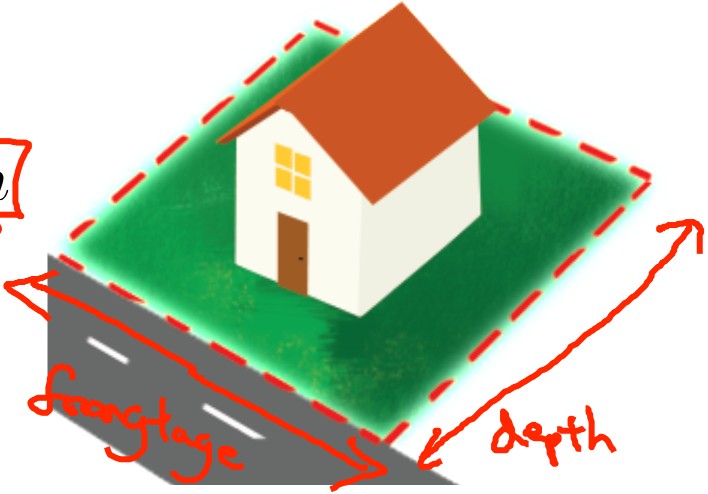
Machine Learning

Linear Regression with multiple variables

Features and polynomial regression

Housing prices prediction

$$h_\theta(x) = \theta_0 + \theta_1 \times \underbrace{\boxed{frontage}}_{\underline{x}_1} + \theta_2 \times \underbrace{\boxed{depth}}_{\underline{x}_2}$$



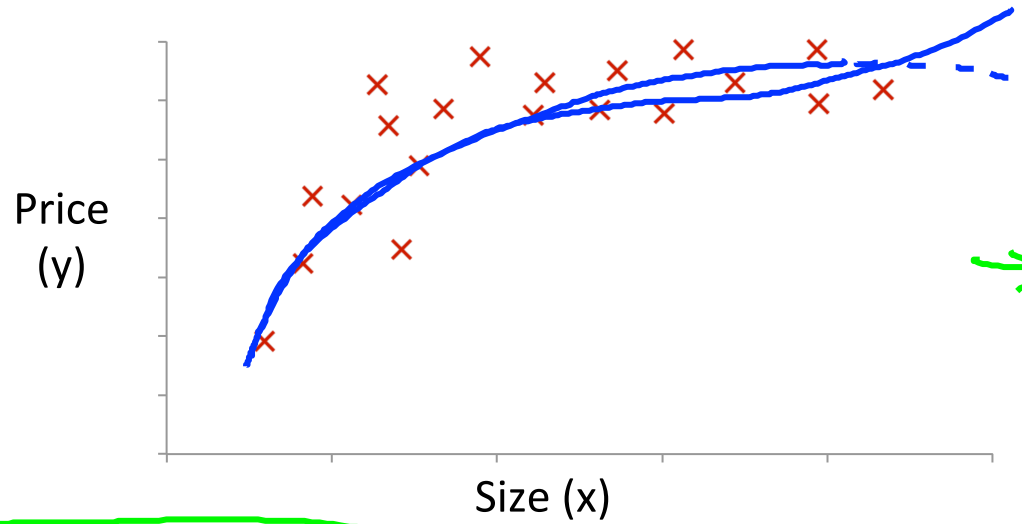
Area

$x = \underline{frontage * depth}$

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

land area

Polynomial regression



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

$$\boxed{\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3}$$

$$\boxed{h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3}$$

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

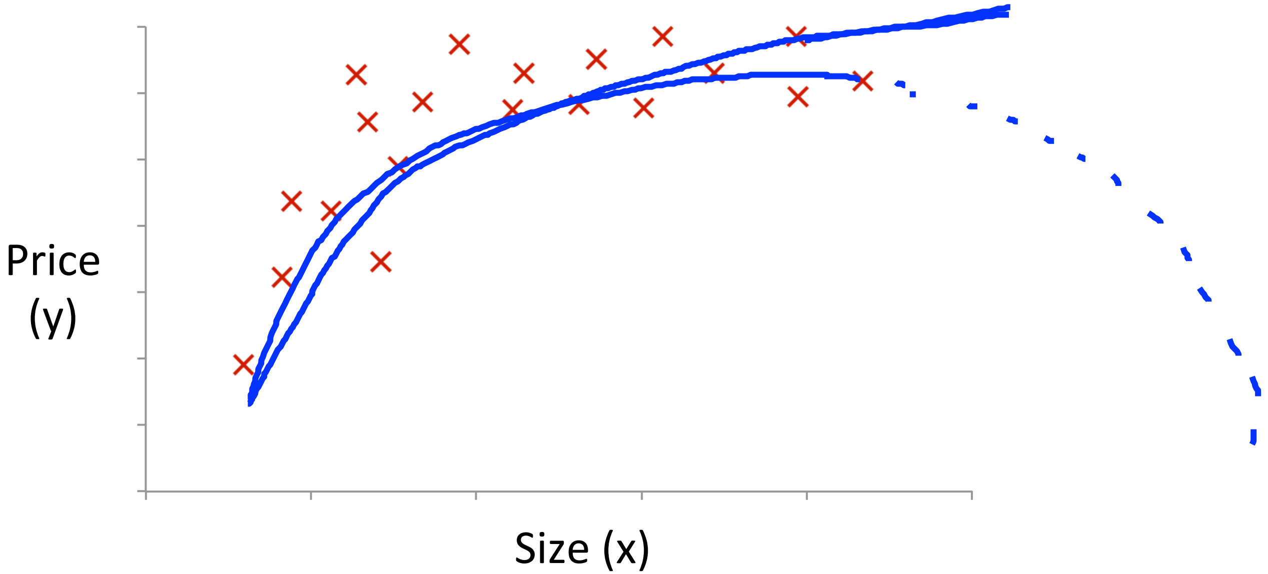
$$x_1 = (size)$$
$$x_2 = (size)^2$$
$$x_3 = (size)^3$$

Size: 1 - 1000

size²: 1 - 1000,000

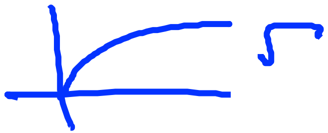
Size³: 1 - 10⁹

Choice of features



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

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



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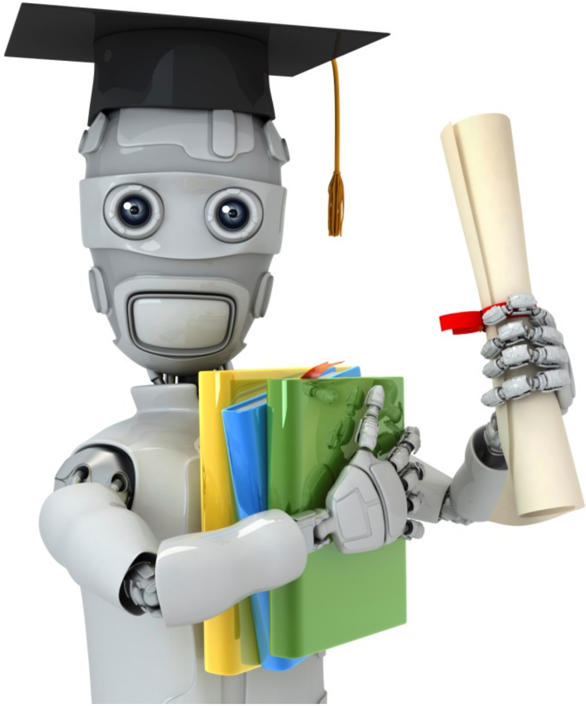
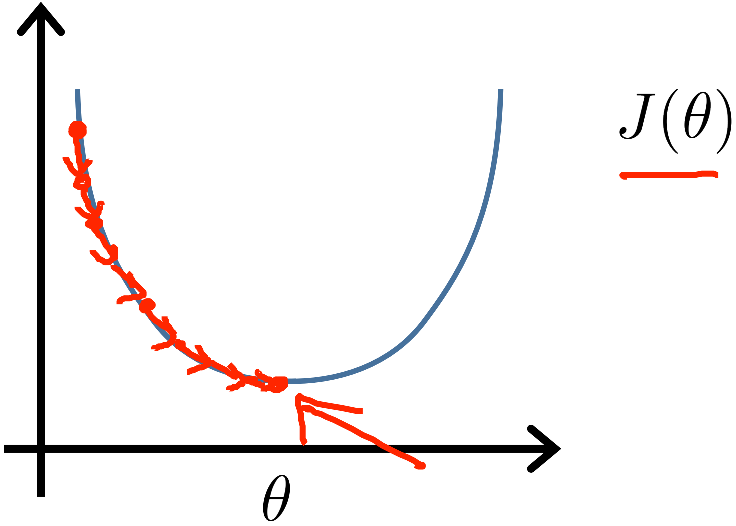


Machine Learning

Linear Regression with multiple variables

Normal equation

Gradient Descent



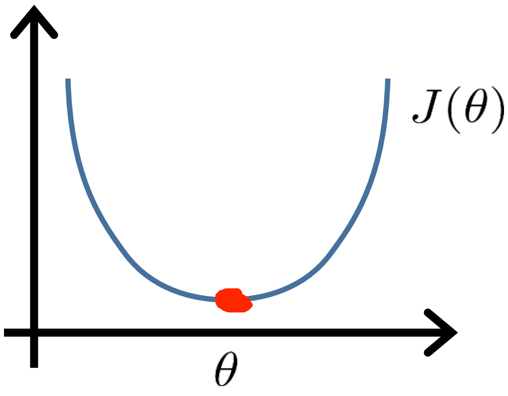
Normal equation: Method to solve for θ analytically.

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

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

$$\frac{\partial}{\partial\theta} J(\theta) = \cdots \overset{\text{set}}{=} 0$$

Solve for θ



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

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

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

Examples: $m = 4.$

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

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

$m \times (n+1)$

m-dimensional vector

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

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

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

$$\underset{\text{(design Matrix)}}{X} = \underbrace{\begin{bmatrix} —— (x^{(1)})^T —— \\ —— (x^{(2)})^T —— \\ \vdots \\ —— (x^{(m)})^T —— \end{bmatrix}}_{m \times (n+1)}$$

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

$$\underline{X} = \underbrace{\begin{bmatrix} 1 & x_1^{(1)} \\ 1 & x_2^{(1)} \\ \vdots & \vdots \\ 1 & x_m^{(1)} \end{bmatrix}}_{m \times 2} \qquad \underline{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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

$$J(\theta)=\frac{1}{2m}\left(X\theta-y\right)^T\left(X\theta-y\right)$$

$$\theta=(X^TX)^{-1}X^Ty:$$

$$\frac{\partial J(\theta)}{\partial \theta_j}=\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^i)-y^i)x_j^i=0(j=0,1,...,n)$$

that's

$$j=0,\begin{bmatrix} h_\theta(x^1)-y^1 \\ \vdots \\ h_\theta(x^n)-y^n \end{bmatrix}^T \begin{bmatrix} x_0^1 \\ \vdots \\ x_0^n \end{bmatrix}=0;\ j=n,\begin{bmatrix} h_\theta(x^1)-y^1 \\ \vdots \\ h_\theta(x^n)-y^n \end{bmatrix}^T \begin{bmatrix} x_n^1 \\ \vdots \\ x_n^n \end{bmatrix}=0$$

$$\Rightarrow \begin{bmatrix} h_\theta(x^1)-y^1 \\ \vdots \\ h_\theta(x^n)-y^n \end{bmatrix}^T \left[\begin{pmatrix} x_0^1 & \cdots & x_n^1 \\ \vdots & \ddots & \vdots \\ x_0^n & \cdots & x_n^n \end{pmatrix}\right]=0 \Rightarrow X^T(X\theta-y)=0$$

$$\Rightarrow \theta=(X^TX)^{-1}X^Ty$$

$$\boxed{\theta = \boxed{(X^TX)^{-1}X^Ty}}$$

$(X^TX)^{-1}$ is inverse of matrix X^TX.

Set $A = X^TX$

$\boxed{(X^TX)^{-1}} = A^{-1}$

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

`pinv(X^T*X)*X^T*y`

$\theta = (X^TX)^{-1}X^Ty$

$\min_\theta J(\theta)$

X' X^T

~~Feature Scaling~~

$0 \le x_1 \le 1$

$0 \le x_2 \le 1000$

$0 \le x_3 \le 10^{-5}$ ✓

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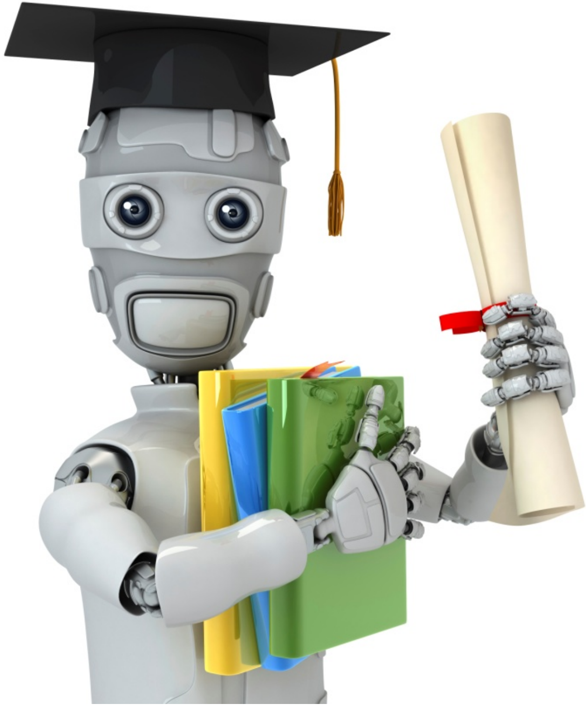
m **training examples,** n **features.**

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



Machine Learning

Linear Regression with multiple variables

Normal equation and non-invertibility (optional)

Normal equation

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

$X^T X$

- What if $\boxed{X^T X}$ is non-invertible? (singular/ degenerate)

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

$\boxed{\text{pinv}}$

inv

What if $\boxed{X^T X}$ is non-invertible?

- Redundant features (linearly dependent).
  E.g. x_1 = size in feet^2
  ~~x_2 = size in m^2~~
  $x_1 = (3.28)^2 x_2$

1m = 3.28 feet

→ $m = 10$ ←
→ $n = 100$ ←
$\theta \in \mathbb{R}^{101}$

- Too many features (e.g. $m \leq n$).
  - Delete some features, or use regularization.

later