





Machine Learning

# Linear Regression with multiple variables

---

## Multiple features

## Multiple features (variables).

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

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

# Multiple features (variables).

Size (feet <sup>2</sup> )	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	36	178
...	...	...	...	...

Notation:

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

$n = 4$

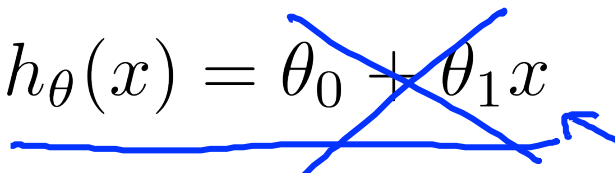
$m = 47$

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

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


Hypothesis:

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



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

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



age

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

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

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

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} \in \mathbb{R}^{n+1}$$

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

$$= \theta^T x$$

$$\begin{bmatrix} \theta_0 & \theta_1 & \dots & \theta_n \end{bmatrix}$$

$\theta^T$

(n+1) x 1  
matrix

$\theta^T x$

$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$x$

Multivariate linear regression.  $\leftarrow$



Machine Learning

# Linear Regression with multiple variables

---

## Gradient descent for multiple variables

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

*Handwritten notes:  $x_0 = 1$  (with arrow pointing to  $x_0$ ),  $\theta$  (underlined),  $n+1$ -dimensional vector*

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

*Handwritten notes:  $\theta$  (underlined),  $n+1$ -dimensional vector*

Cost function:

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

*Handwritten notes:  $J(\theta)$  (underlined),  $J(\theta)$  (underlined)*

Gradient descent:

Repeat {

$\rightarrow \theta_j := \theta_j - \alpha \left[ \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n) \right]$

*Handwritten notes:  $J(\theta)$  (underlined),  $J(\theta)$  (underlined)*

}

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

# Gradient Descent

Previously ( $n=1$ ):

Repeat {

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

→  $\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_1^{(i)}$   
(simultaneously update  $\theta_0, \theta_1$ )

}

New algorithm ( $n \geq 1$ ):

Repeat {

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

(simultaneously update  $\theta_j$  for  $j = 0, \dots, n$ )

}

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

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

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

...





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.  $x_1 = \text{size (0-2000 feet}^2\text{)}$  ←

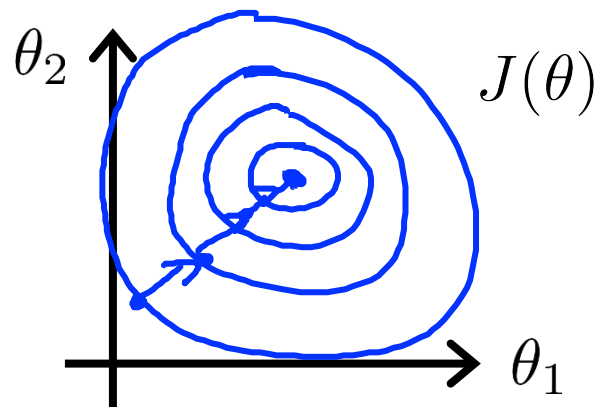
$x_2 = \text{number of bedrooms (1-5)}$  ←



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

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

$$0 \leq x_1 \leq 1 \quad 0 \leq x_2 \leq 1$$



## Feature Scaling

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

$$x_0 = 1$$

$$0 \leq x_1 \leq 3 \quad \checkmark$$

$$-2 \leq x_2 \leq 0.5 \quad \checkmark$$

$$-100 \leq x_3 \leq 100 \quad \times$$

$$-0.0001 \leq x_4 \leq 0.0001 \quad \times$$

$$-3 \text{ to } 3 \quad \checkmark$$

$$-\frac{1}{3} \text{ to } \frac{1}{3} \quad \checkmark$$

# 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.  $\rightarrow x_1 = \frac{\text{size} - 1000}{2000}$

Average size = 1000

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

1-5 bedrooms

$$\rightarrow [-0.5 \leq x_1 \leq 0.5, -0.5 \leq x_2 \leq 0.5]$$

$$x_1 \leftarrow \frac{x_1 - \mu_1}{S_1}$$

← avg value of  $x_1$  in training set

range (max-min)  
(or standard deviation)

$$x_2 \leftarrow \frac{x_2 - \mu_2}{S_2}$$



Machine Learning

# Linear Regression with multiple variables

---

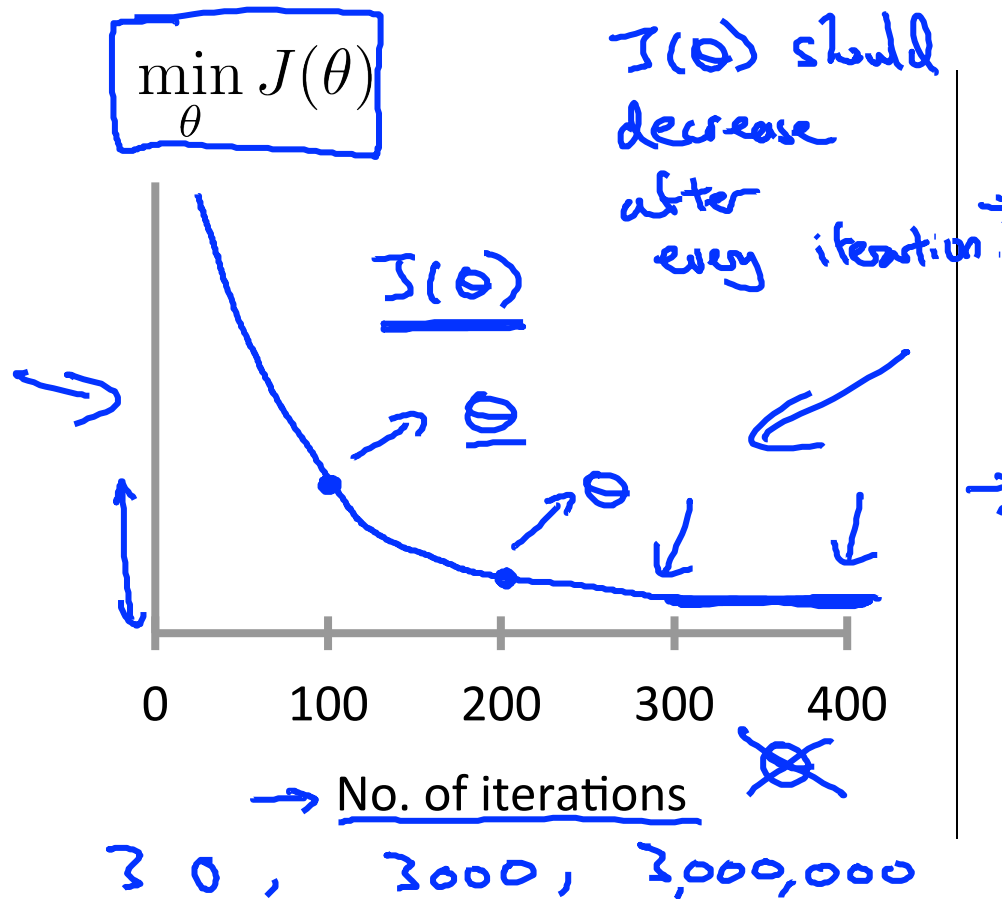
Gradient descent in practice II: Learning rate

# Gradient descent

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

- “Debugging”: How to make sure gradient descent is working correctly.
- How to choose learning rate  $\alpha$ .

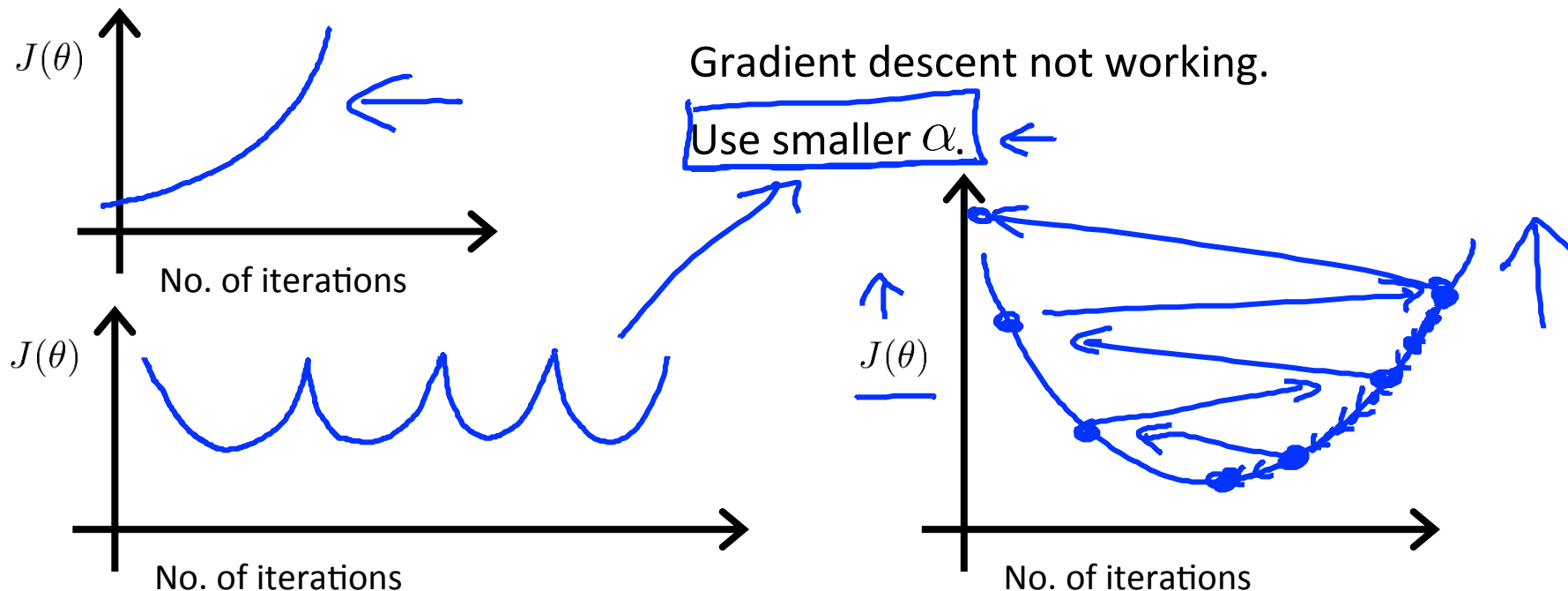
# Making sure gradient descent is working correctly.



→ Example automatic convergence test:

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

# Making sure gradient descent is working correctly.



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



## Summary:

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



To choose  $\alpha$ , try

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

Arrows indicate the sequence of values, with labels  $\approx 3\times$  and  $\approx 10\times$  indicating the relative increase in  $\alpha$  between consecutive values.



Machine Learning

# Linear Regression with multiple variables

---

Features and  
polynomial regression

# Housing prices prediction

$$h_{\theta}(x) = \theta_0 + \theta_1 \times \underbrace{\text{frontage}}_{x_1} + \theta_2 \times \underbrace{\text{depth}}_{x_2}$$

Area

$$x = \underline{\text{frontage} \times \text{depth}}$$

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

↖ land area



# Polynomial regression



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

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

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

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

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

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

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

Size: 1-1000

Size<sup>2</sup>: 1-1,000,000

Size<sup>3</sup>: 1-10<sup>9</sup>

# Choice of features



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

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





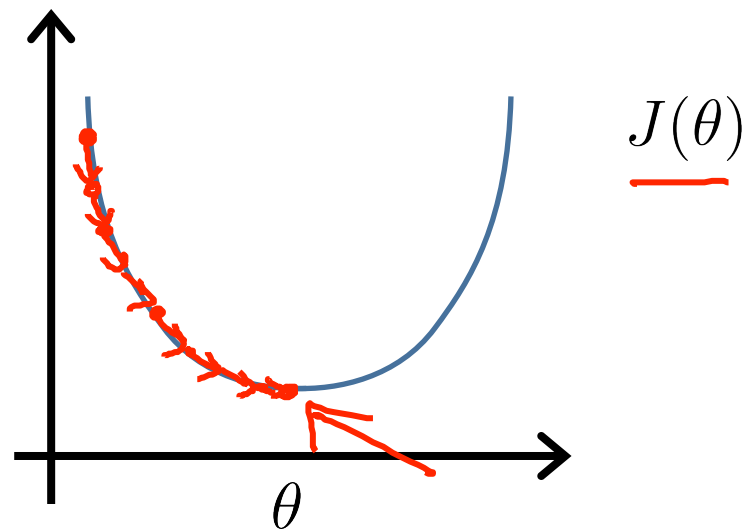
Machine Learning

# Linear Regression with multiple variables

---

## Normal equation

# Gradient Descent



Normal equation: Method to solve for  $\theta$   
analytically.

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

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

$\frac{\partial}{\partial \theta} J(\theta) = \dots \stackrel{\text{set}}{=} 0$

Solve for  $\theta$



---

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

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

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



Examples:  $m = 4$ .

	Size (feet <sup>2</sup> )	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

$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}$   
 $m \times (n+1)$

$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$   
 $m$ -dimensional vector

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

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

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

$X$   
(design matrix)

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

$m \times (n+1)$

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

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

$$\begin{bmatrix} 1 & x_1^{(1)} \\ 1 & x_1^{(2)} \\ \vdots & \vdots \\ 1 & x_1^{(m)} \end{bmatrix} \quad \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

$m \times 2$

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

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

Set  $A = X^T X$

$$(X^T X)^{-1} = A^{-1}$$

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

$$\text{pinv}(X^T * X) * X^T * y$$

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

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

$X'$	$X^T$
	<del>Feature Scaling</del>
	$0 \leq x_1 \leq 1$
	$0 \leq x_2 \leq 1000$
	$0 \leq x_3 \leq 10^{-5}$ ✓

$m$  training examples,  $n$  features.

### Gradient Descent

- • Need to choose  $\alpha$ .
- • Needs many iterations.
- Works well even when  $n$  is large.

↗  
 $n = 10^6$

← -

### Normal Equation

- • No need to choose  $\alpha$ .
- • Don't need to iterate.
- Need to compute
- •  $(X^T X)^{-1}$   $n \times n$   $O(n^3)$
- 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

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

$$\underline{X^T X}$$

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

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

$\theta$

$\boxed{\text{pinv}}$   
inv

What if  $X^T X$  is non-invertible?

- Redundant features (linearly dependent).

E.g.  $x_1 = \text{size in feet}^2$

~~$x_2 = \text{size in m}^2$~~

$$x_1 = (3.28)^2 x_2$$

$$1\text{m} = 3.28\text{ feet}$$

$$\rightarrow m = 10 \leftarrow$$

$$\rightarrow n = 100 \leftarrow$$

$$\theta \in \mathbb{R}^{101}$$

- Too many features (e.g.  $m \leq n$ ).

- Delete some features, or use regularization.

↓ later