





Machine Learning

Linear Regression with multiple variables

Multiple features

Multiple features (variables).

Size (feet ²)	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 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
...

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. $\underline{h_0(x)} = \underline{80} + \underline{0.1x_1} + \underline{0.01x_2} + 3x_3 - 2x_4$
↑ ↑ ↑
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 $x_0 = 1$. ($x_0^{(i)} = 1$)

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

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

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

$$= \theta^T x$$

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

θ^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), θ (underlined), $n+1$ -dimensional vector

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

Handwritten notes: θ (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 {

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

→ $\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \underline{x_1^{(i)}}$
(simultaneously update θ_0, θ_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 θ_j for $j = 0, \dots, n$)

}

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

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

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

...



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

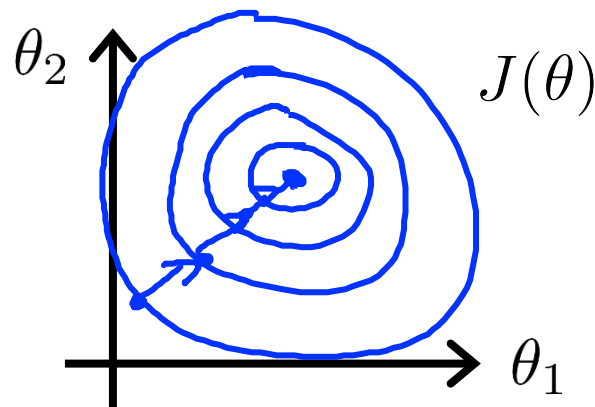
$x_2 = \text{number of bedrooms (1-5)}$ ←



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

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

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



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

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

$$x_1 \leftarrow \frac{x_1 - \mu_1}{\sigma_1}$$

← avg value of x_1 in training set

range (max-min)
(or standard deviation)

$$x_2 \leftarrow \frac{x_2 - \mu_2}{\sigma_2}$$



Machine Learning

Linear Regression with multiple variables

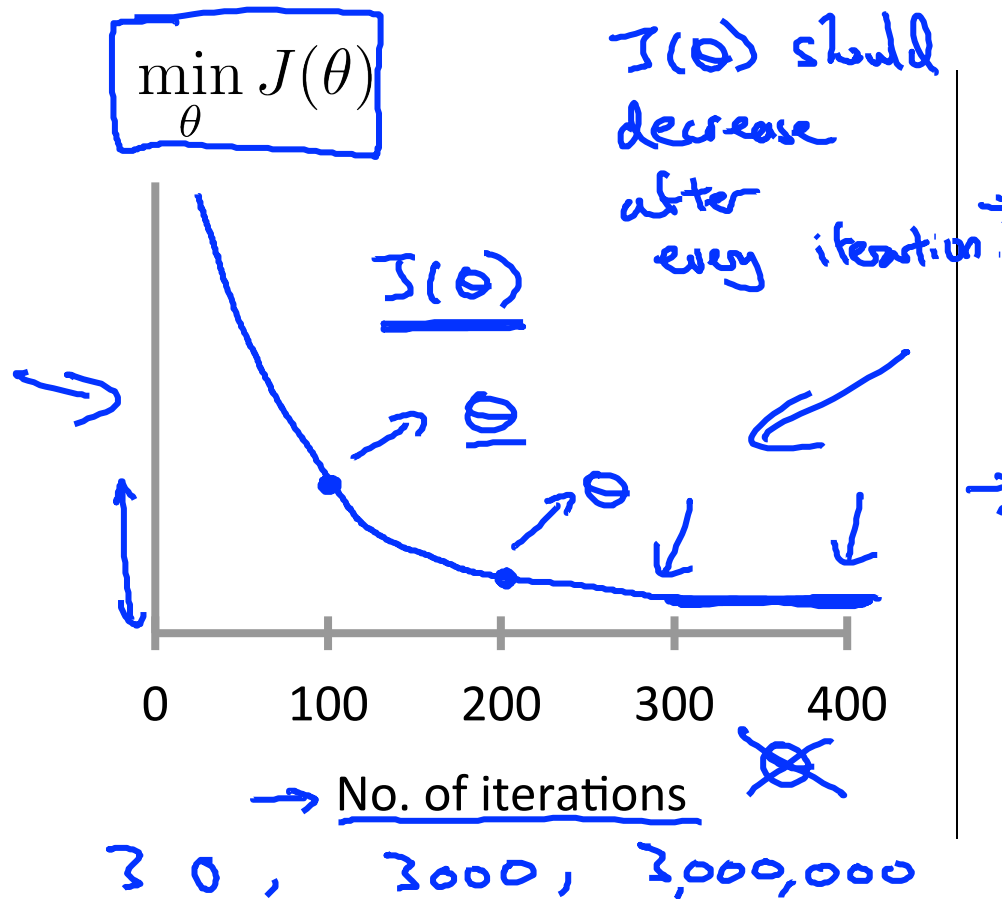
Gradient descent in practice II: Learning rate

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 α .

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 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

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

Handwritten blue annotations below the sequence of values: upward arrows point to 0.001, 0.03, 0.1, and 1. Curved arrows connect 0.001 to 0.003, 0.003 to 0.01, 0.01 to 0.03, and 0.03 to 0.1. Each of these curved arrows is labeled with $\approx 3\times$, indicating a threefold increase in the step size 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

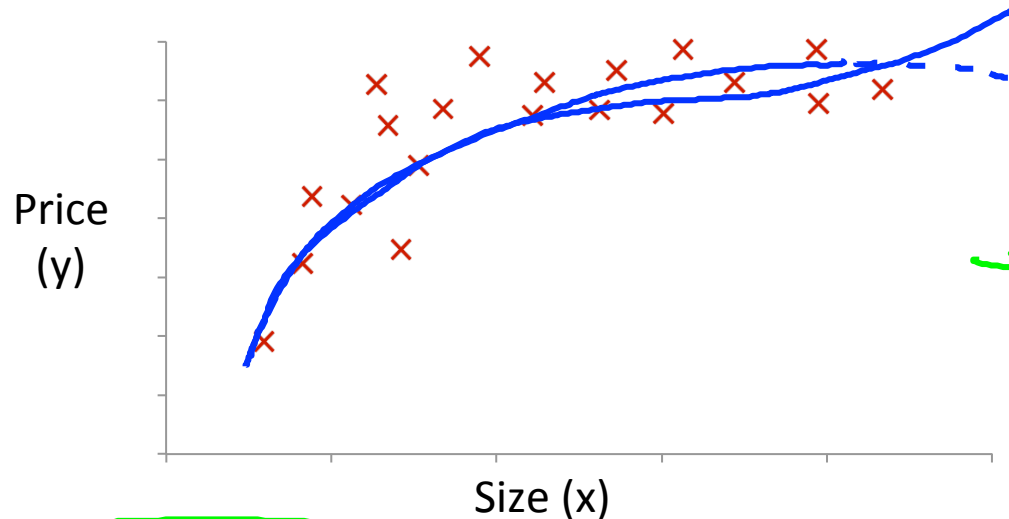
$$x = \underline{\text{frontage} \times \text{depth}}$$

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

↖ 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

Size²: 1-1,000,000

Size³: 1-10⁹

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



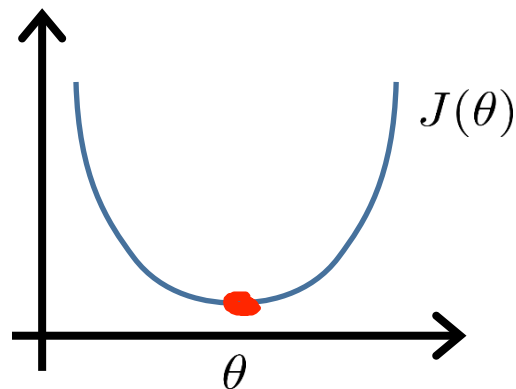
Normal equation: Method to solve for θ
analytically.

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 θ



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

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

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

Examples: $m = 4$.

	Size (feet ²)	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
	Feature Scaling
	$0 \leq x_1 \leq 1$
	$0 \leq x_2 \leq 1000$
	$0 \leq x_3 \leq 10^{-5}$ ✓

m training examples, n features.

Gradient Descent

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

↗
 $n = 10^6$

← -

Normal Equation

- • No need to choose α .
- • 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`

θ

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

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

- Redundant features (linearly dependent).

E.g. $\begin{cases} \underline{x_1} = \text{size in feet}^2 \\ \underline{x_2} = \text{size in m}^2 \\ \underline{x_1 = (3.28)^2 x_2} \end{cases}$

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

$$\rightarrow m = 10 \leftarrow$$

$$\rightarrow n = 100 \leftarrow$$

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

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

- Delete some features, or use regularization.

↓ later