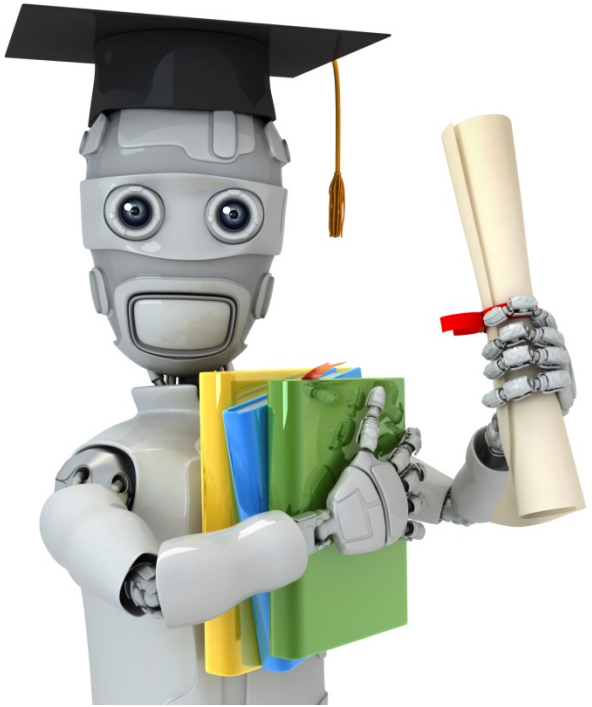


Machine Learning

Linear Regression with multiple variables

Multiple features

Multiple features (variables).

original case, we only consider size of the house one variable

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.

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

$x_3^{(2)} = 2$

Hypothesis:

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

new hypothesis

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

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

x_2 ↑

x_3 ↑

x_4 ↑ age

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

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

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

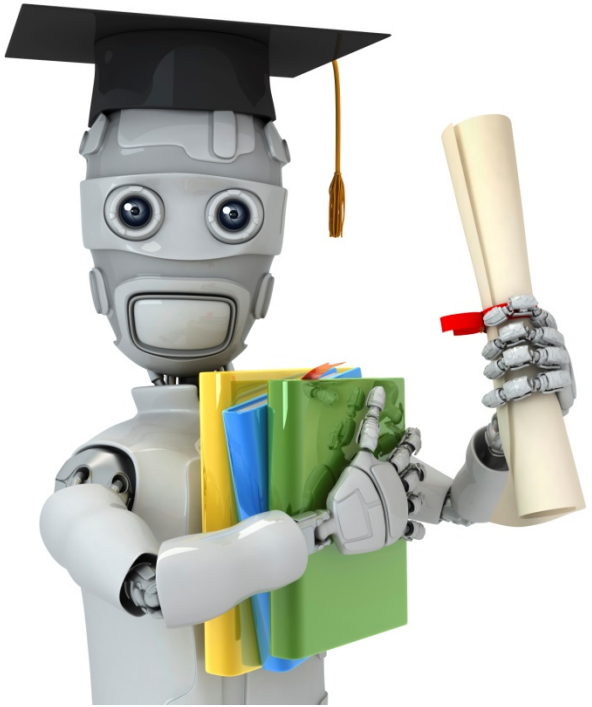
$[\theta_0\ \theta_1 \cdots \theta_n]$ = θ^T, $(n+1) \times 1$ matrix

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

$= \theta^T x$

$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$ ($x_0 = 1$)

Multivariate linear regression.



Machine Learning

Linear Regression with multiple variables

Gradient descent for multiple variables

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

$x_0 = 1$

Parameters: $\theta_0, \theta_1, \ldots, \theta_n$ θ

n+1 - dimensional vector

Cost function:

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

$J(\theta)$

Gradient descent:

Repeat $\{$

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \ldots, \theta_n)$$

$J(\theta)$

$\}$

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

Gradient Descent

Previously (n=1):

Repeat $\{$

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

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

(simultaneously update θ_0, θ_1)

$\}$

New algorithm $(n \geq 1)$:

Repeat $\{$

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

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

$\}$

$x_0^{(i)} = 1$

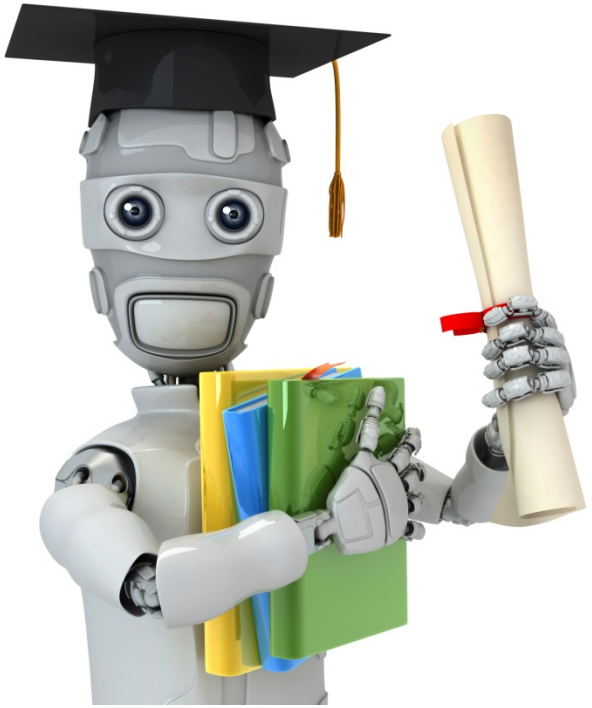
Consider we have two features, thus three parameters

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

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

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

...



Machine Learning

Linear Regression with multiple variables

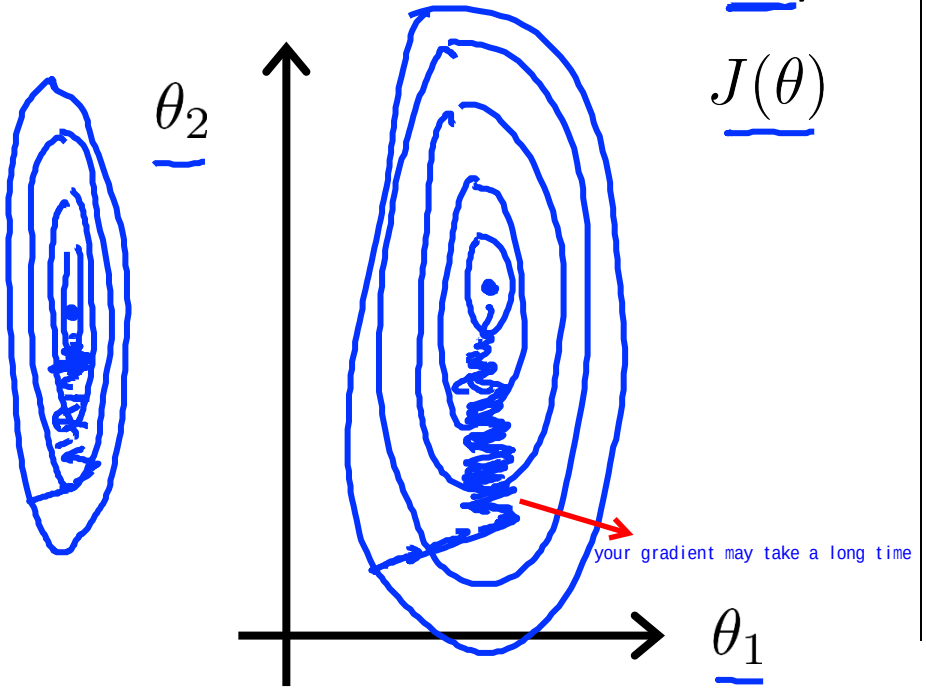
Gradient descent in practice I: Feature Scaling

Feature Scaling

Idea: Make sure features are on a similar scale. we scale features, apples to apples comparison

E.g. x_1 = size (0-2000 feet²)

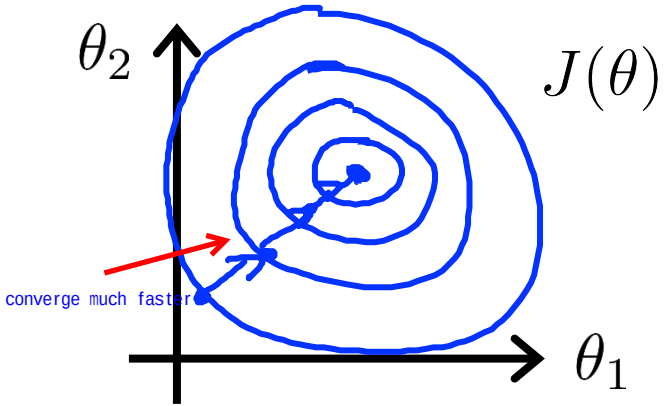
x_2 = number of bedrooms (1-5)



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

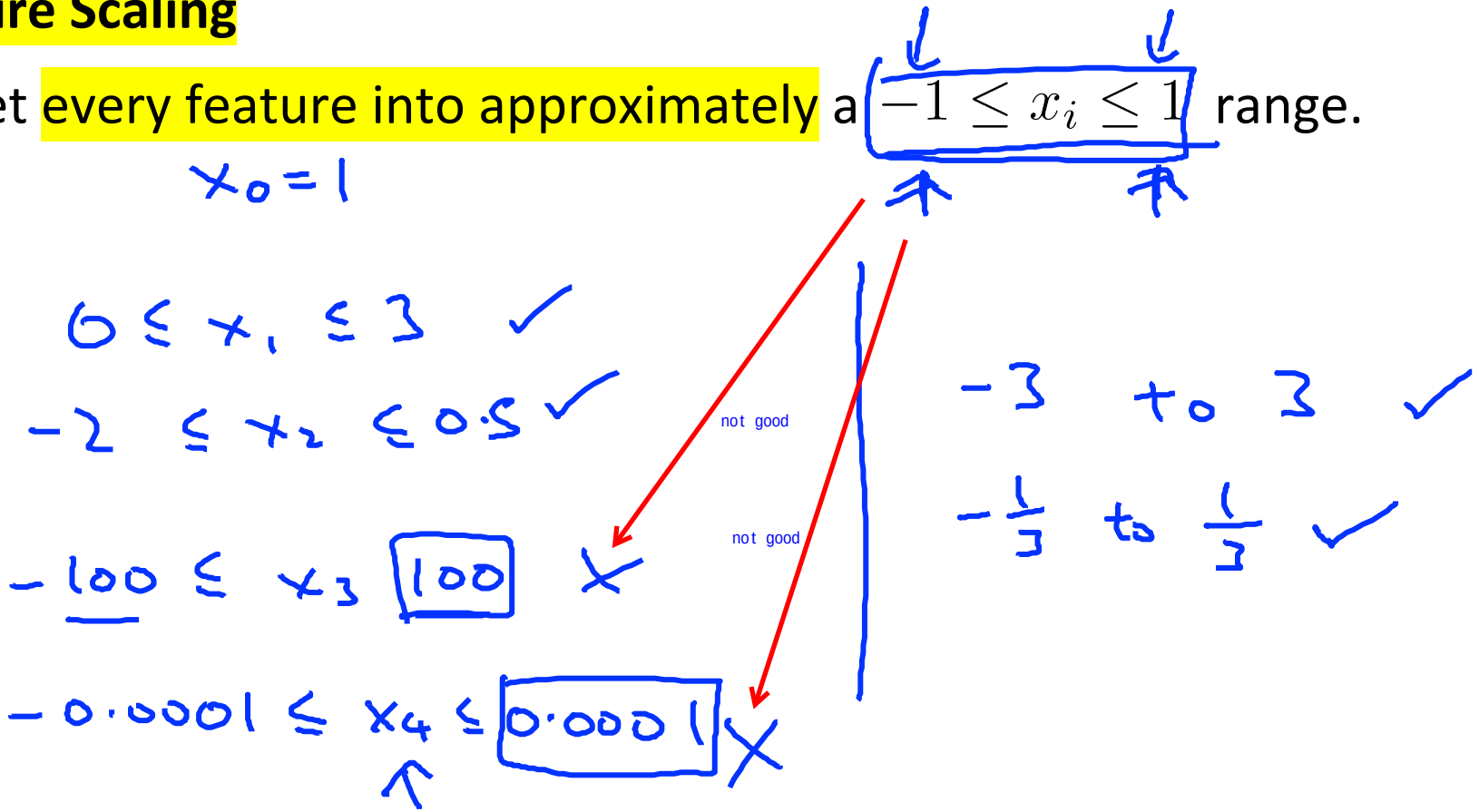
$$x_2 = \frac{\text{number of bedrooms}}{5}$$

$0 \le x_1 \le 1$ $0 \le x_2 \le 1$



Feature Scaling

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



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

Average size = 100

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

1-5 bedrooms

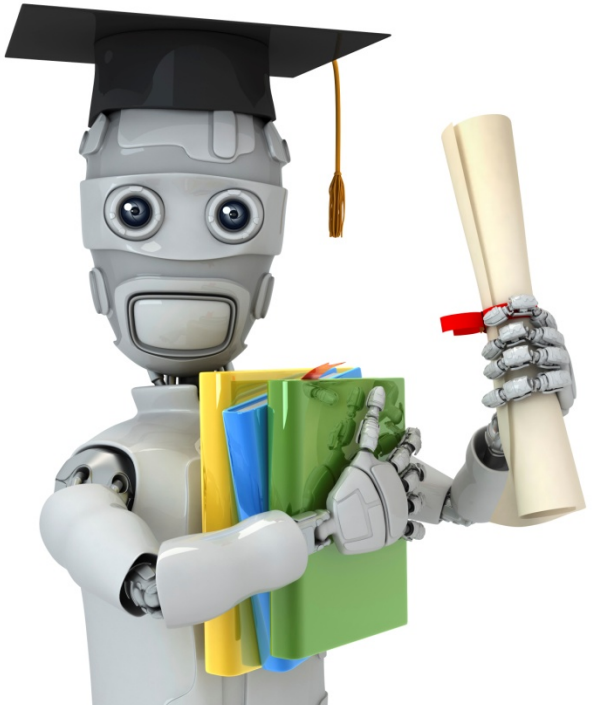
$-0.5 \leq x_1 \leq 0.5$, $-0.5 \leq x_2 \leq 0.5$

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

range (max - min)

(or standard deviation)

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



Machine Learning

Linear Regression with multiple variables

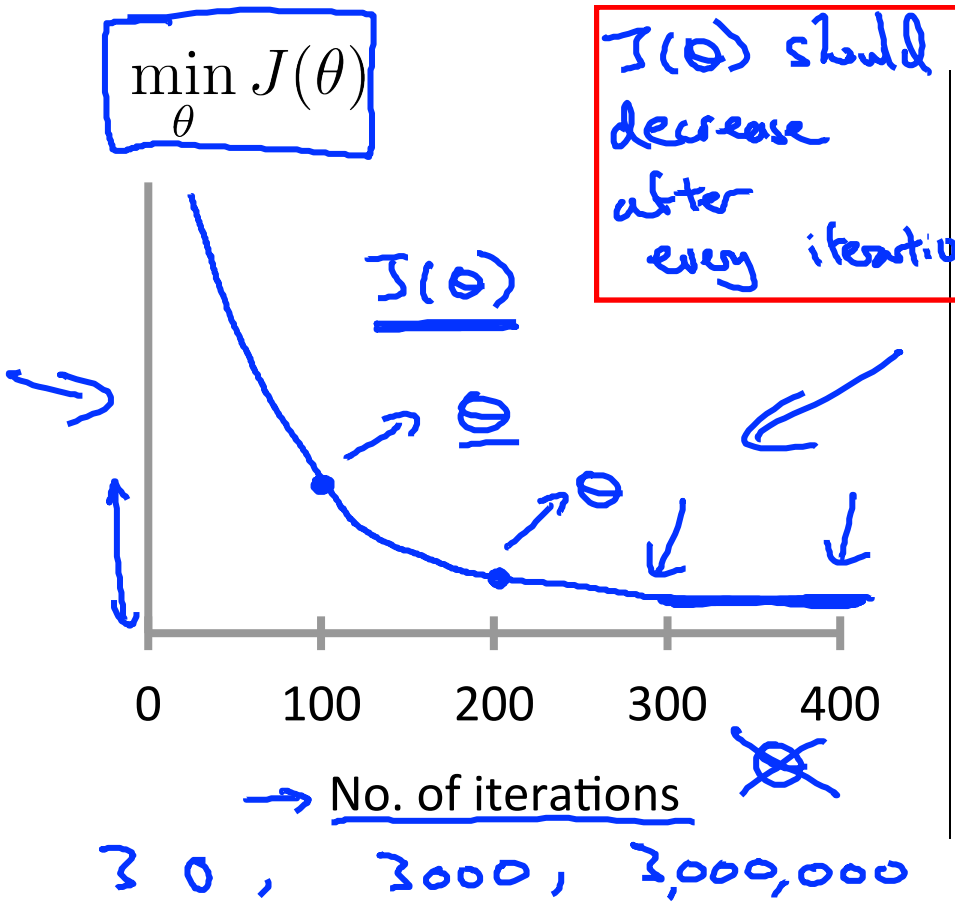
Gradient descent in practice II: Learning rate

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 α.

Making sure gradient descent is working correctly.



should decrease

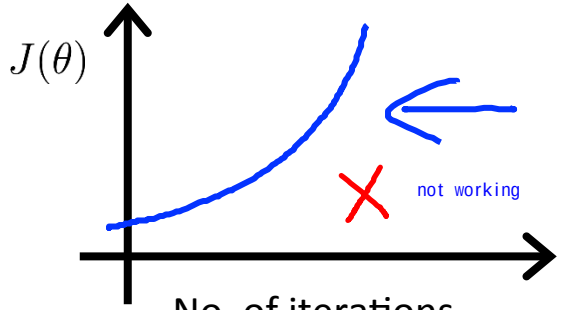
Example automatic convergence test:

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

ε

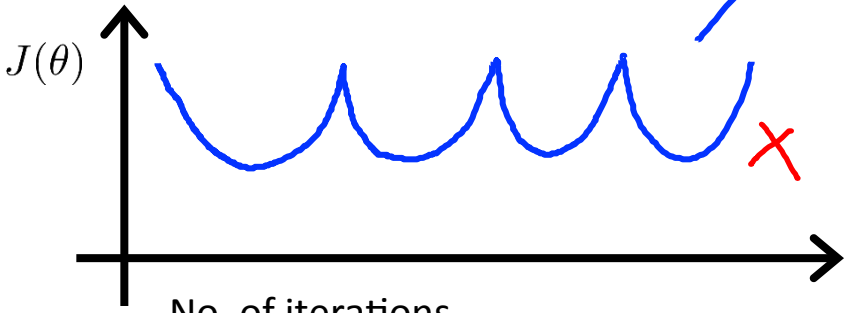
some small value

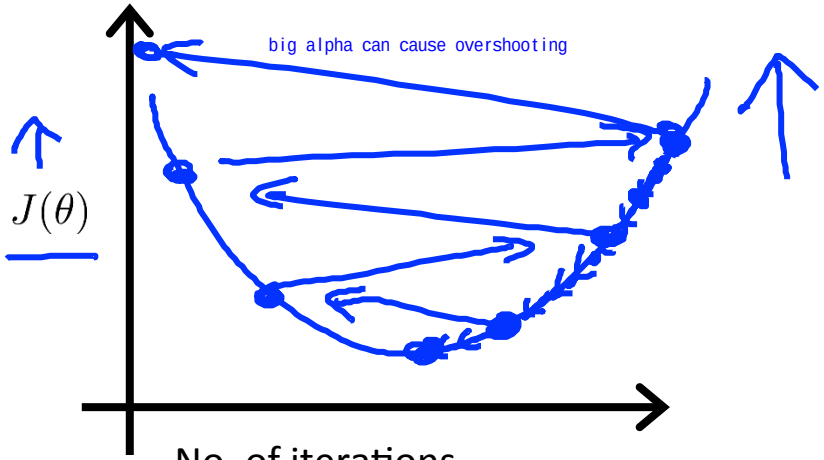
Making sure gradient descent is working correctly.



Gradient descent not working.

Use smaller α.

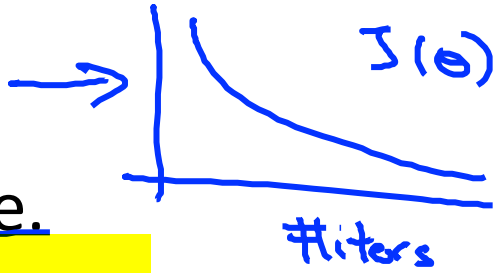




math people have theoretically proved!

- 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:

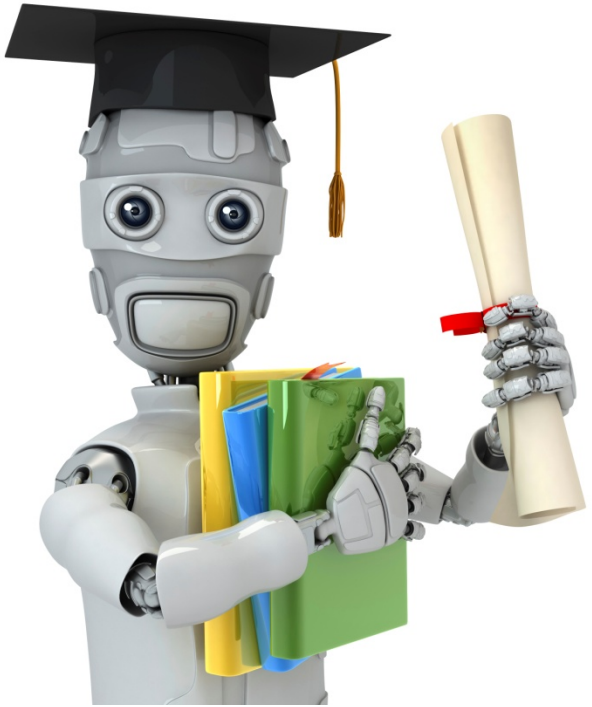


- If α is too small: slow convergence.
- If α is too large: $J(\theta)$ may not decrease on every iteration; may not converge. (Slow converge also possible)

To choose α, try

try a range of alphas

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



Machine Learning

Linear Regression with multiple variables

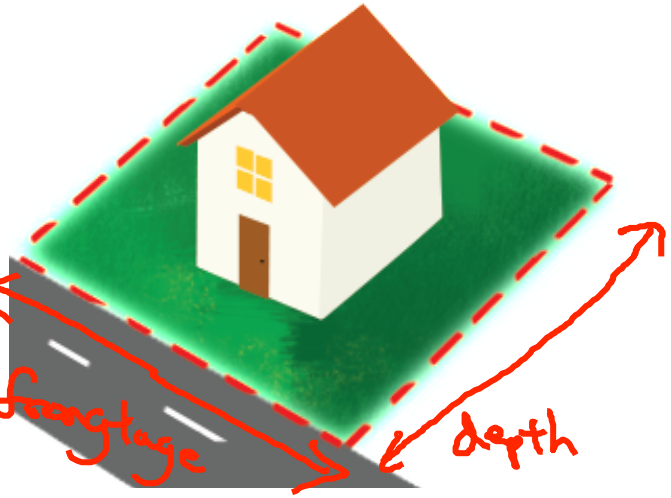
Features and polynomial regression

Housing prices prediction

two features

$$h_\theta(x) = \theta_0 + \theta_1 \times frontage + \theta_2 \times depth$$

x_1 x_2



Area

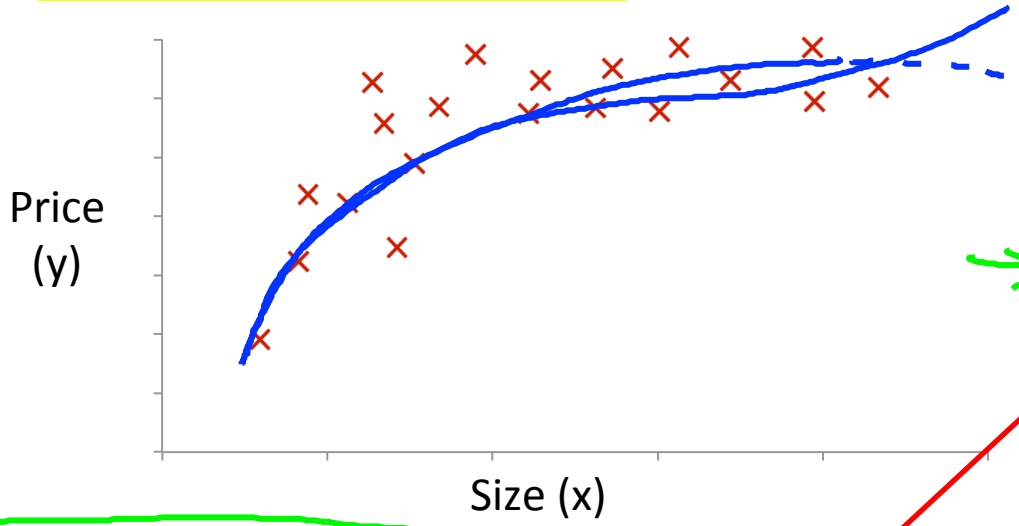
x = frontage * depth

we can create a new feature

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

↑ land area

Polynomial regression



choose your features

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

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

fit the cubic model

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$
$$= \theta_0 + \theta_1 (size) + \theta_2 (size)^2 + \theta_3 (size)^3$$

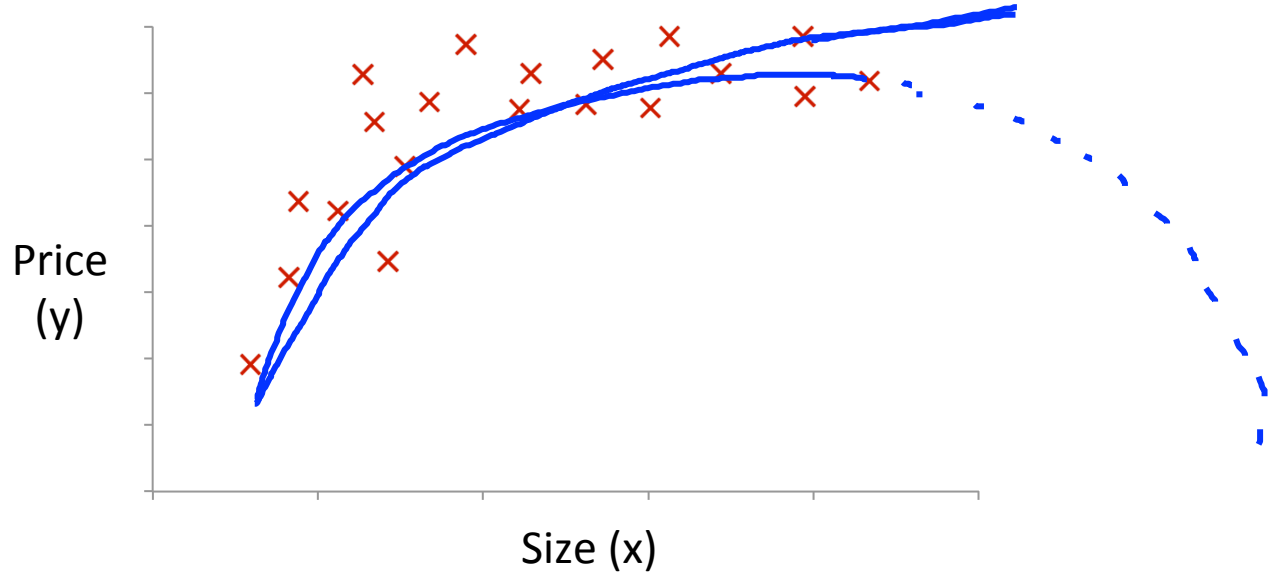
$$x_1 = (size)$$
$$x_2 = (size)^2$$
$$x_3 = (size)^3$$

Size: 1 - 1000

Size^2: 1 - 1000,000

Size^3: 1 - 10^9

Choice of features



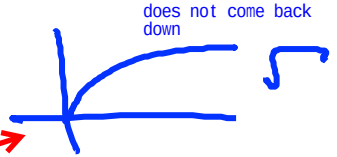
quadratic/cubic candidate

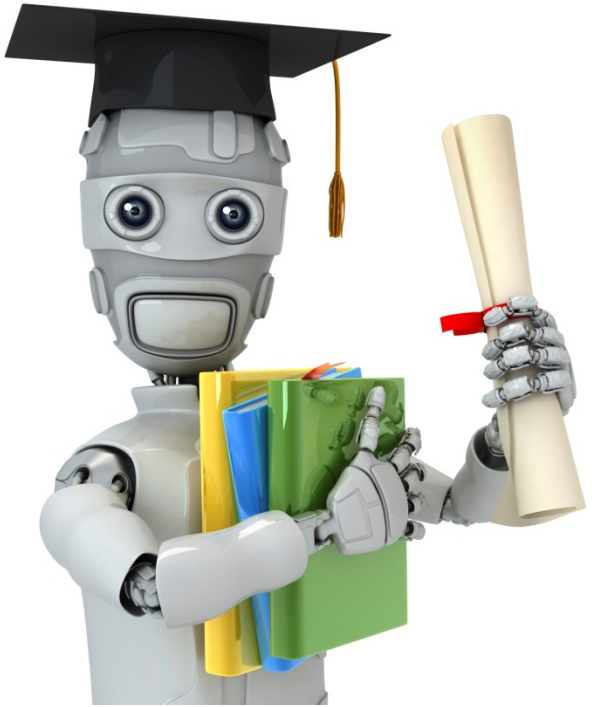
$$h_\theta(x) = \theta_0 + \theta_1(size) + \theta_2(size)^2$$

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

another reasonable choice

does not come back down





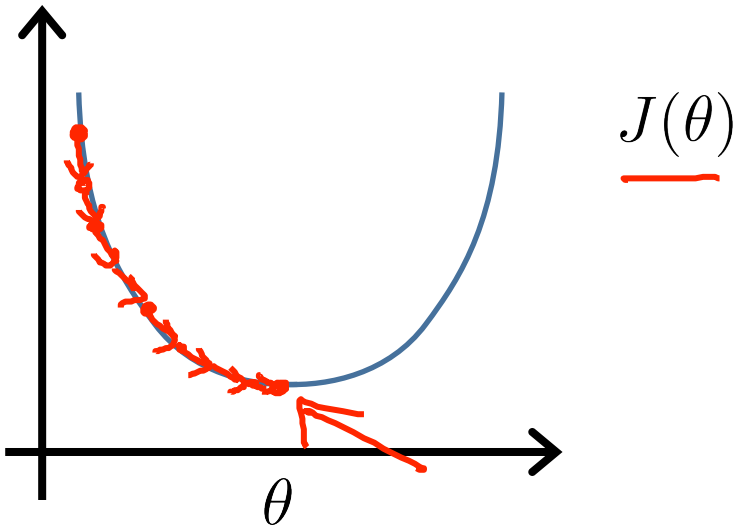
Machine Learning

Linear Regression with multiple variables

Normal equation

Analytically solve the problem/pseudo inverse

Gradient Descent



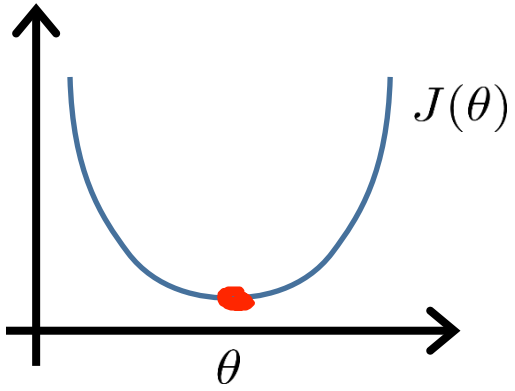
Normal equation: Method to solve for θ analytically.

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

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

$\frac{d}{d\theta} J(\theta) = \cdots$ set 0

Solve for θ



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

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

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

analytical solution from calculus

Examples: $m = 4$.

x_0	Size (feet^2) 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

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}$$

$m \times (n+1)$

$y = X\theta$

$$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

m-dimensional vector

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

pseudo inverse of X

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

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

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 $x^{(i)} = \begin{bmatrix} 1 \\ x_1^{(i)} \end{bmatrix}$

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

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

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

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

Set $A = X^T X$

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

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

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

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

$\min_\theta J(\theta)$

X' X^T

~~Feature Scaling~~

feature scaling is not a problem

$0 \le x_1 \le 1$

$0 \le x_2 \le 1000$

$0 \le x_3 \le 10^{-5}$ ✓

m training examples, n features.

very useful!!!

Gradient Descent

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

$n = 10^6$ definitely using gradient descent

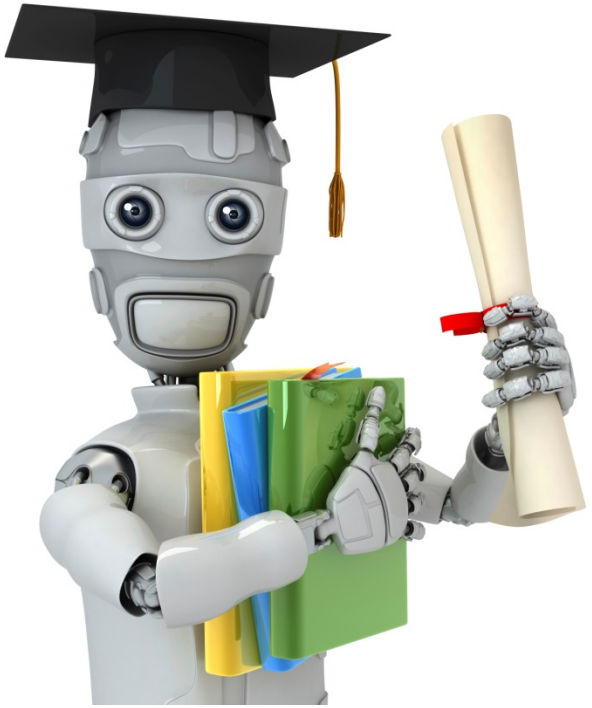
Normal Equation

- No need to choose α.
- Don't need to iterate.
- Need to compute $(X^T X)^{-1}$ $n \times n$ $O(n^3)$ requires computation
- Slow if n is very large.

$n = 100$ ✓

$n = 1000$ ✓

$n = 10000$ may consider gradient descent



Machine Learning

Linear Regression with multiple variables

Normal equation and non-invertibility (optional)

Normal equation

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

- What if $X^T X$ is non-invertible? (singular/ degenerate)
- Octave: `pinv(X'*X)*X'*y`

pseudo inverse

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

- Redundant features (linearly dependent).
  E.g. x_1 = size in feet^2
  x_2 = size in m^2
  $x_1 = (3.28)^2 x_2$
  $1\text{m} = 3.28$ feet
- Too many features (e.g. $m \leq n$).
  $m = 10$
  $n = 100$
  $\in \mathbb{R}^{101}$
  - Delete some features, or use regularization.
    ↓ later