ФИСТ
УлГТУ

Robotics & Data Mining Summer School

Lesson 04. Basics of Machine Learning

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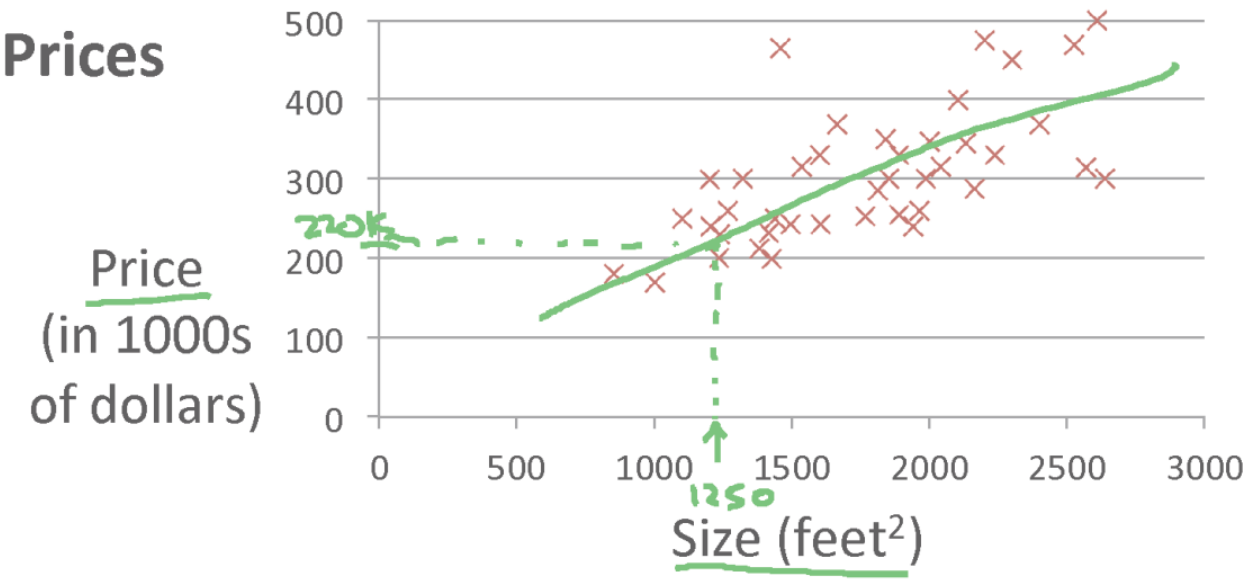
Linear regression with one variable

Model representation

Housing Prices



Supervised Learning

Given the "right answer" for each example in the data.

Regression Problem

Predict real-valued output

Classification: Discrete-valued output

Training set of housing prices (Portland, OR)

Size in feet^2 (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
...	...

m = 47

Notation:

- **m** = Number of training examples
- **x**'s = "input" variable / features
- **y**'s = "output" variable / "target" variable

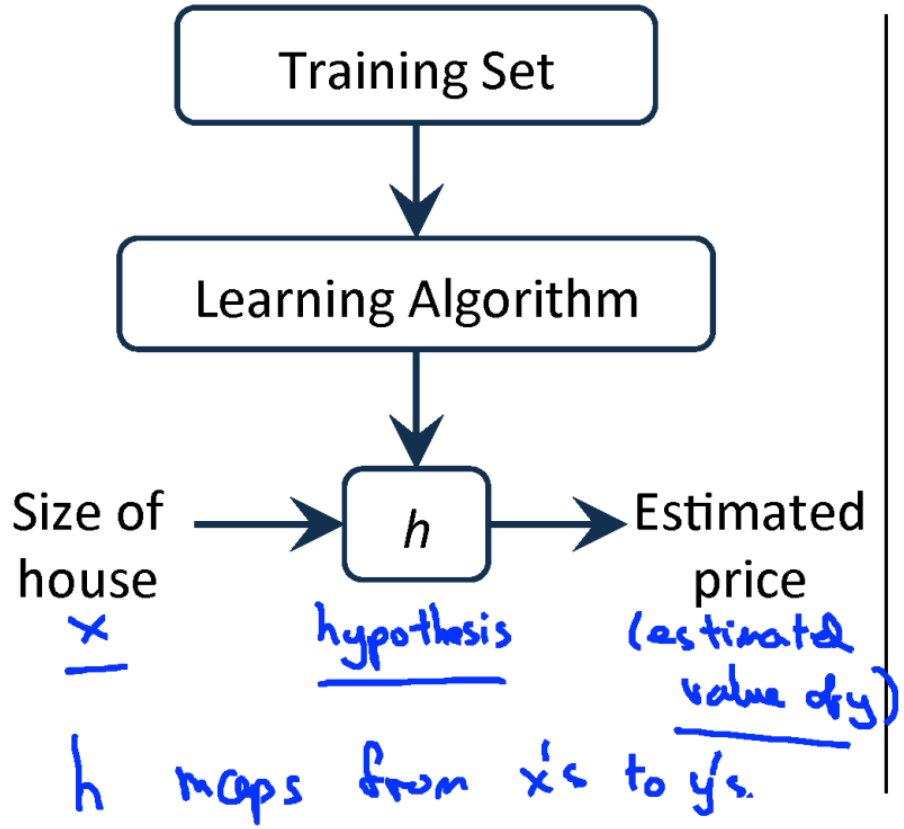
(x, y) - one training example

$(x^{(i)}, y^{(i)})$ - i^{th} training example

$x^{(1)} = 2104$

$x^{(2)} = 1416$

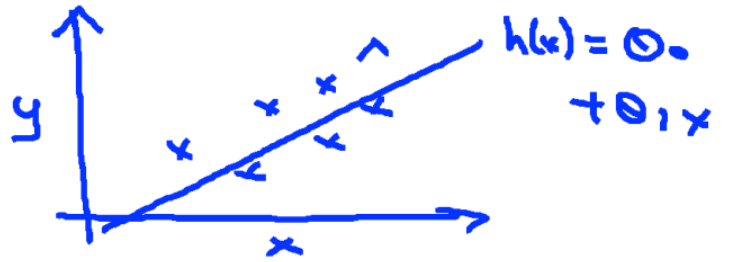
$y^{(1)} = 460$



How do we represent *h* ?

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

Shorthand: $h(x)$



Linear regression with one variable. (x)

Univariate linear regression.

└ one variable

Cost function

Training Set

Size in feet^2 (x)	Price ($) in 1000's (y)
2104	460
1416	232
1534	315
852	178
...	...

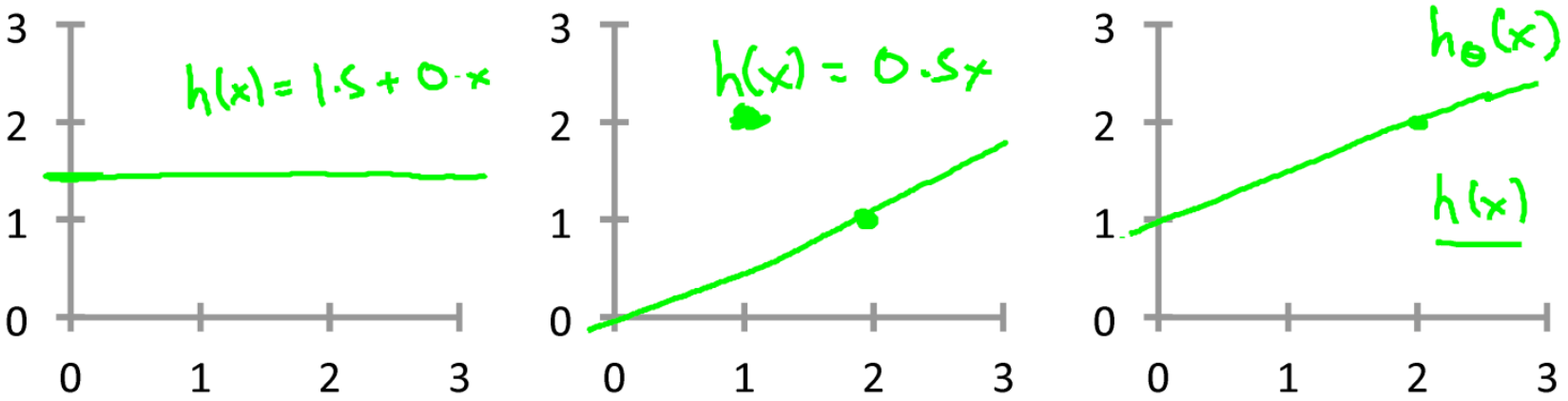
$m = 47$

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

θ_i's: Parameters

How to choose θ_i's ?

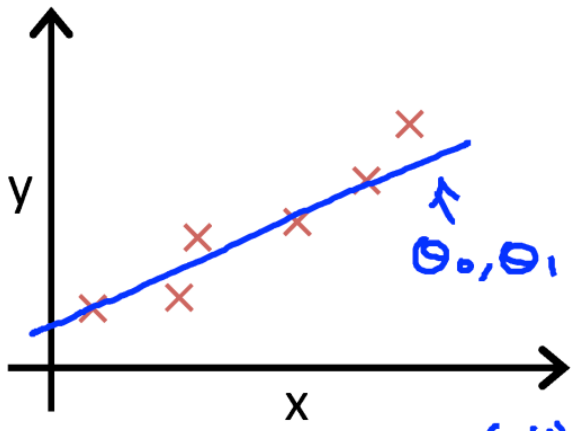
$$h_\theta(x) = \theta_0 + \theta_1 x$$



- $\theta_0 = 1.5$
- $\theta_1 = 0$

- $\theta_0 = 0$
- $\theta_1 = 0.5$

- $\theta_0 = 1$
- $\theta_1 = 0.5$



#training examples

$$\text{minimize}_{\theta_0,\theta_1} \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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

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

Idea: Choose θ_0, θ_1 so that $h_\theta(x)$ is close to y for our training examples (x, y)

x, y

Minimize $J(\theta_0,\theta_1)$
θ_0,θ_1

Cost function

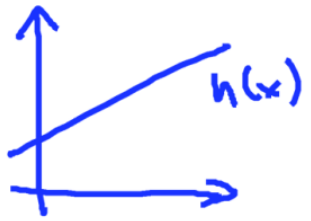
Squared error function

Hypothesis:

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

Parameters:

$$\theta_0, \theta_1$$



Cost Function:

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

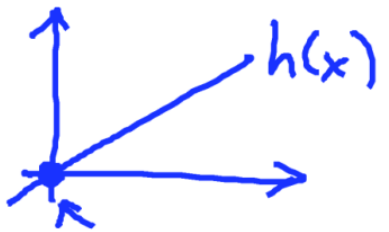
Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

Simplified

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

$\theta_0 = 0$

θ_1



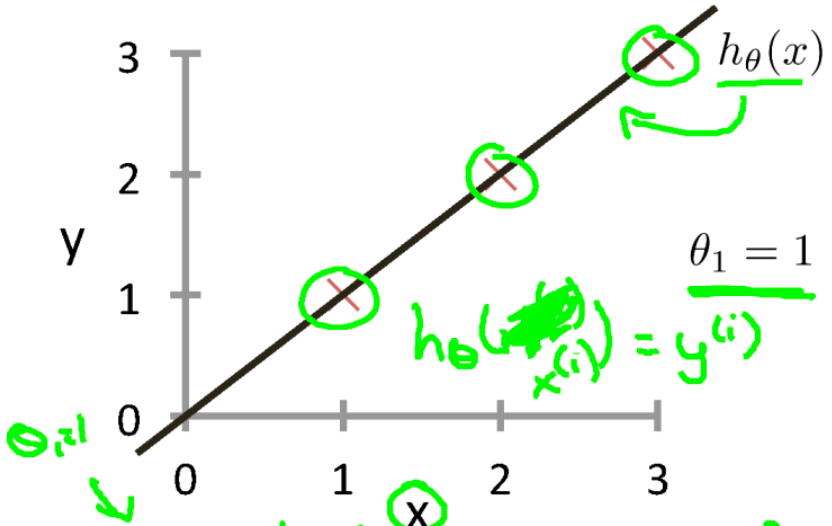
$$J(\theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$\theta, x^{(i)}$

$\underset{\theta_1}{\text{minimize}}\ J(\theta_1)$

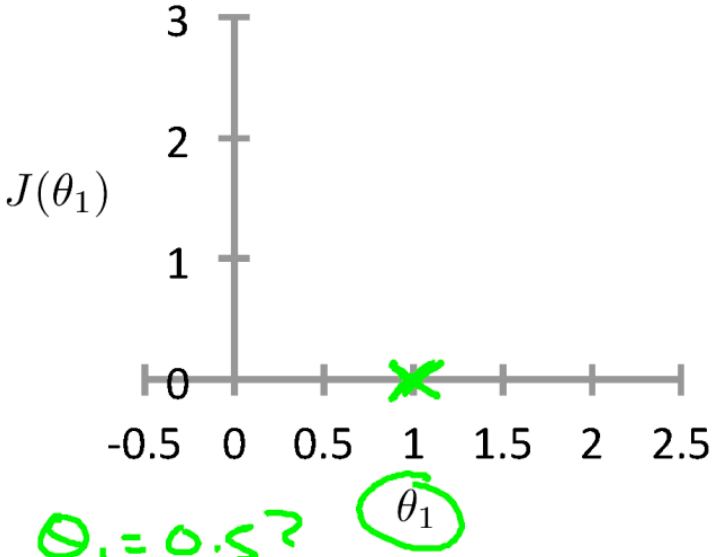
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)



$h_\theta(x^{(i)}) = y^{(i)}$

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

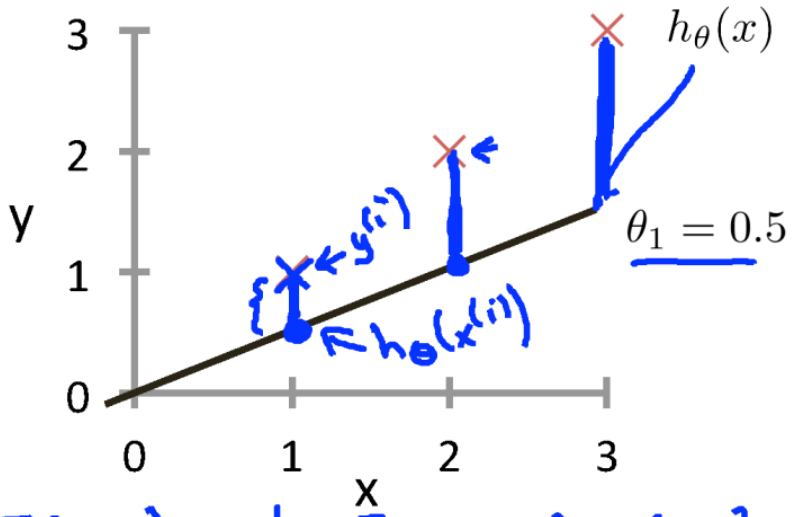
$= \frac{1}{2m} \sum_{i=1}^{m} (\theta_1 x^{(i)} - y^{(i)})^2 = \frac{1}{2m}(0^2 + 0^2 + 0^2) = 0^2$

$\theta_1 = 0.5$?

$J(1) = 0$

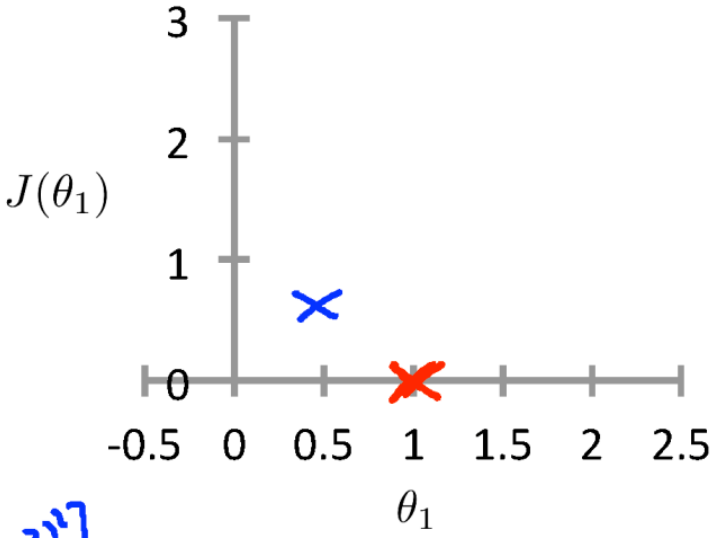
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)



$J(0.5) = \frac{1}{2m}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right]$

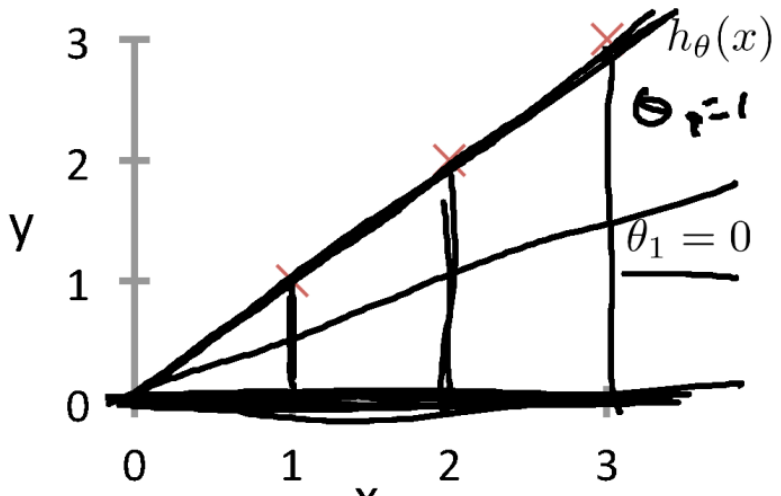
$= \frac{1}{2\times 3}(3.5) = \frac{3.5}{6} \approx 0.58$

$\theta_1 = 0?$

$J(0) = ?$

$h_\theta(x)$

(for fixed θ_1, this is a function of x)

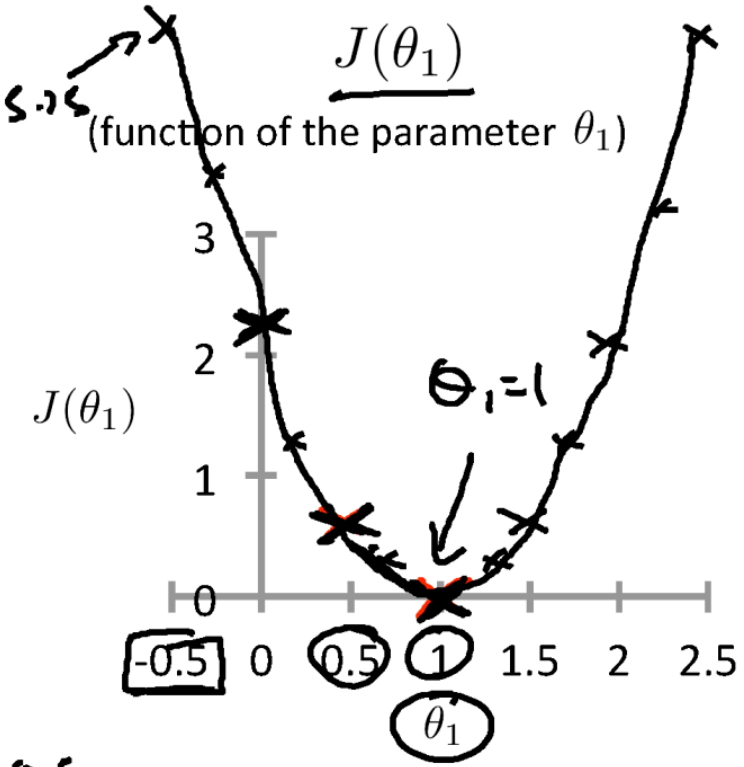


$J(0) = \frac{1}{2m}(1^2 + 2^2 + 3^2)$

$= \frac{1}{6}(14) \approx 2.3$

$J(\theta_1)$

(function of the parameter θ_1)



$h(x) = -0.5$

Minimize $J(\theta_1)$

θ_1

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

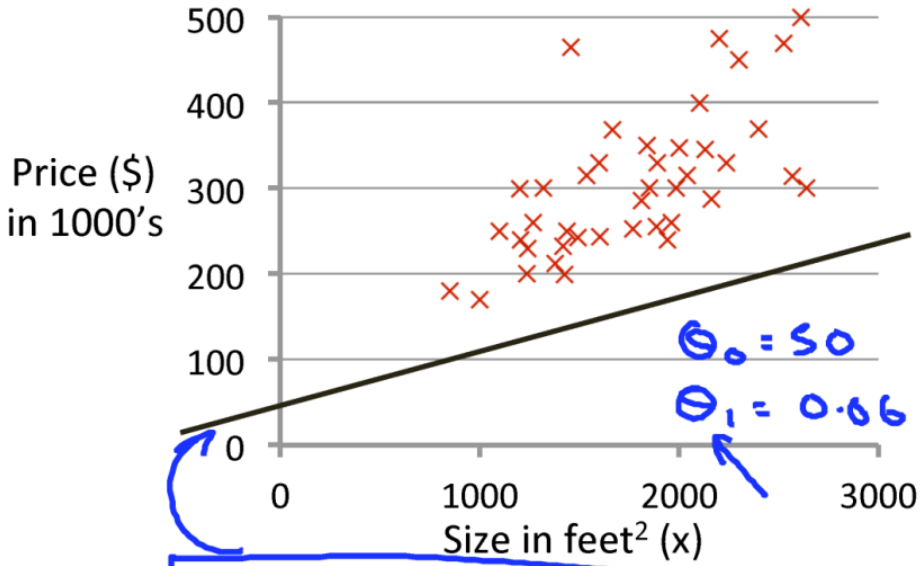
Parameters: θ_0, θ_1

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

Goal: $\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$

$h_\theta(x)$

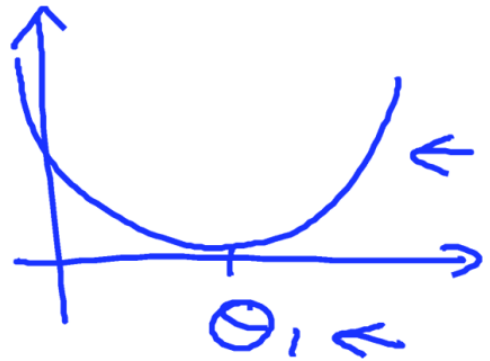
(for fixed θ_0, θ_1, this is a function of x)



$h_\theta(x) = 50 + 0.06x$

$J(\theta_0, \theta_1)$

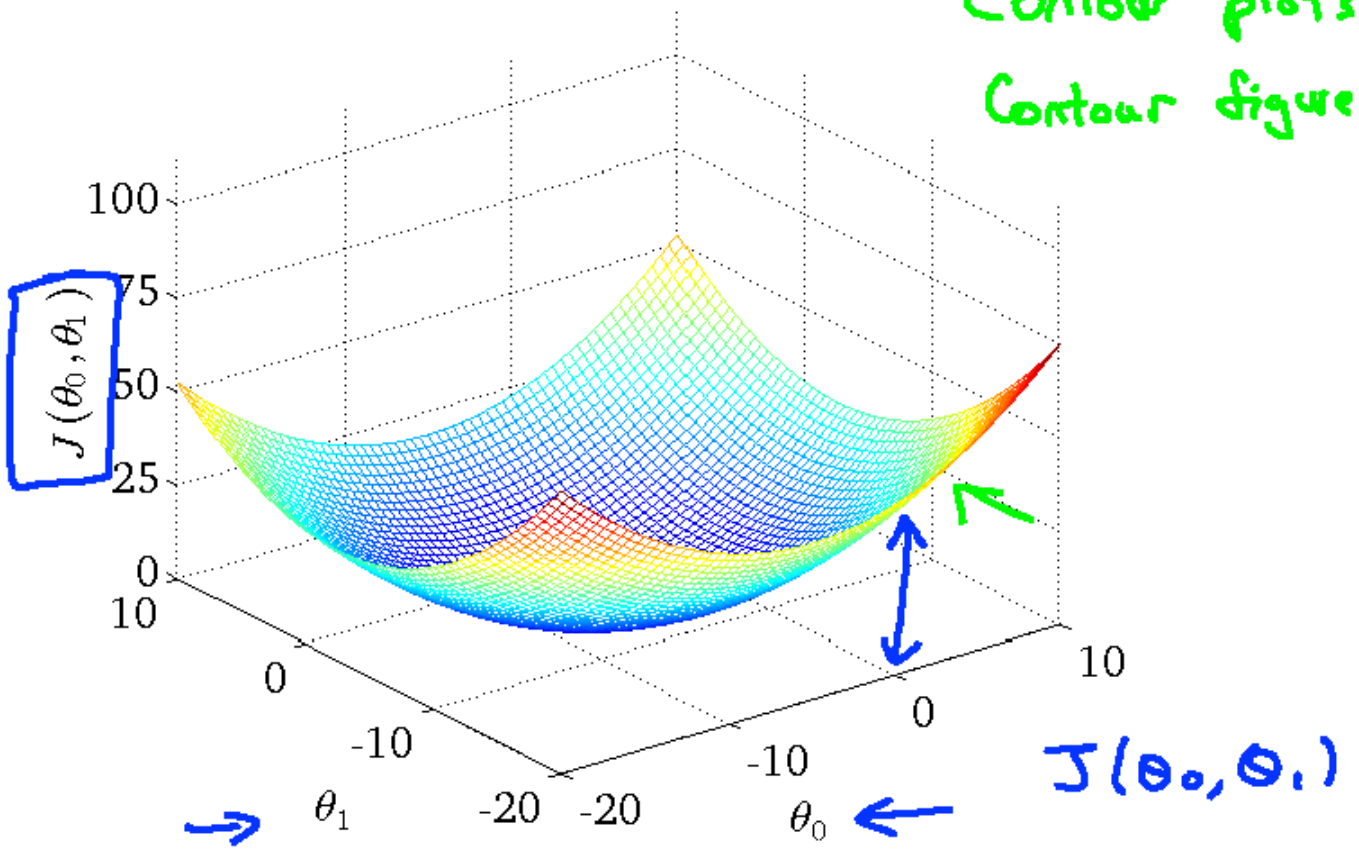
(function of the parameters θ_0, θ_1)



θ_0, θ_1

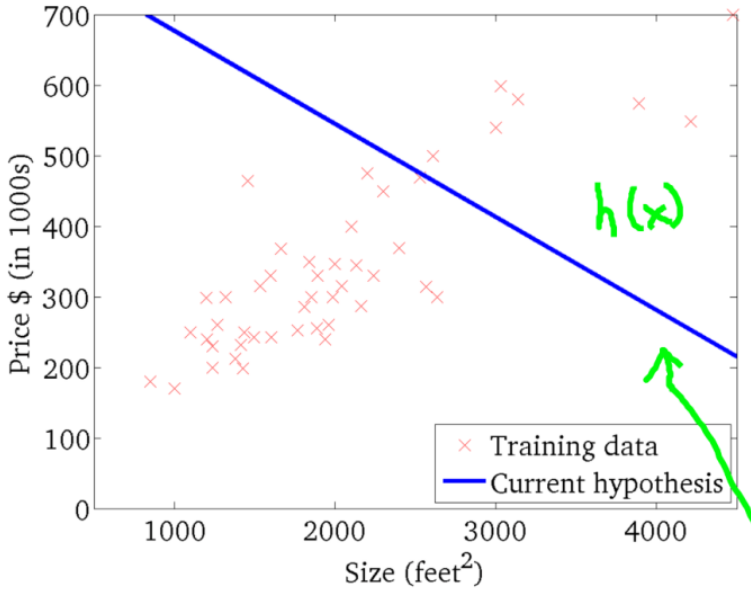
Contour plots

Contour figures -



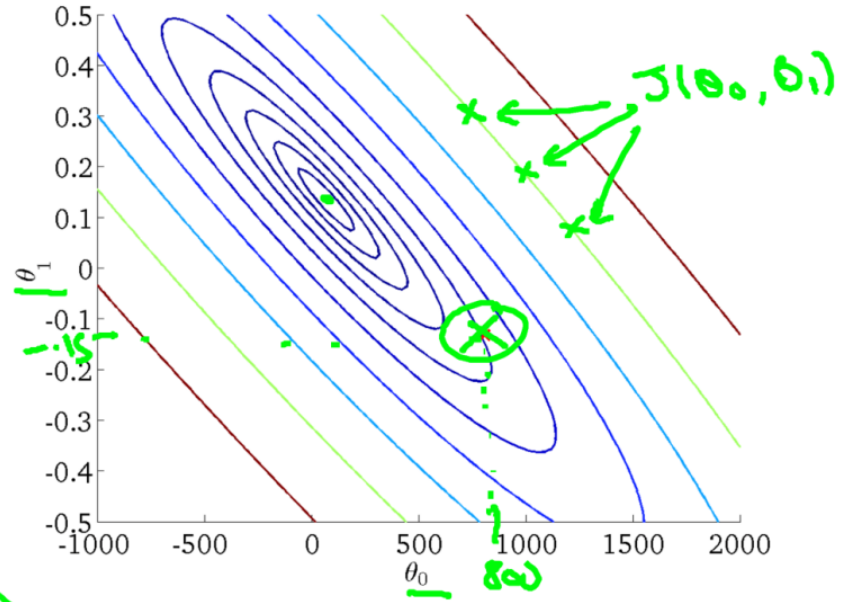
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



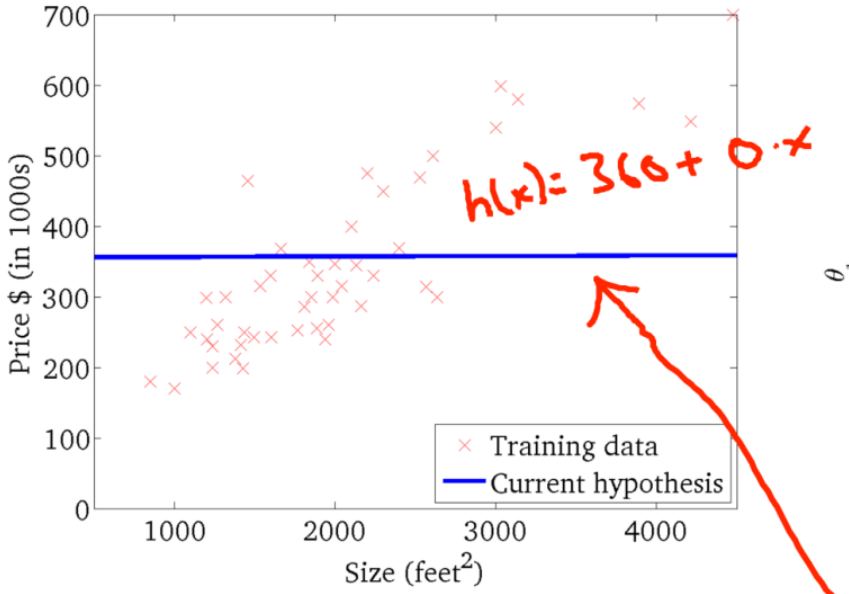
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



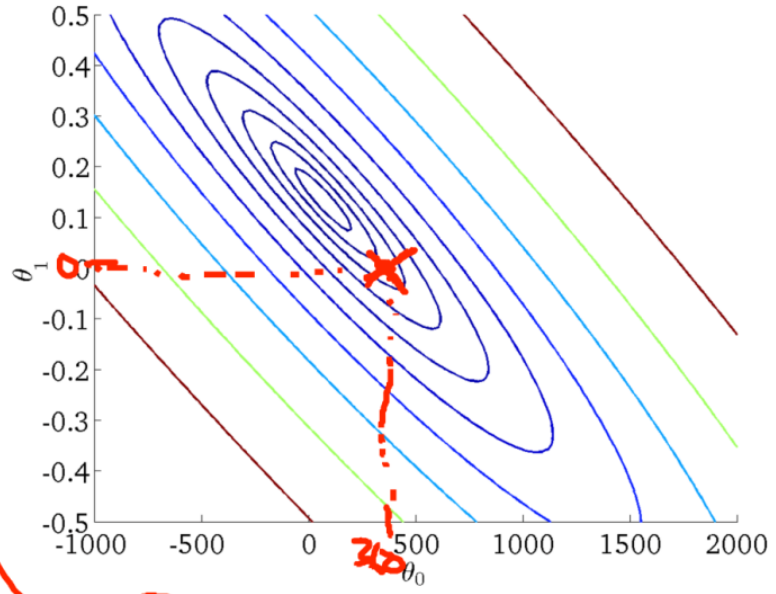
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



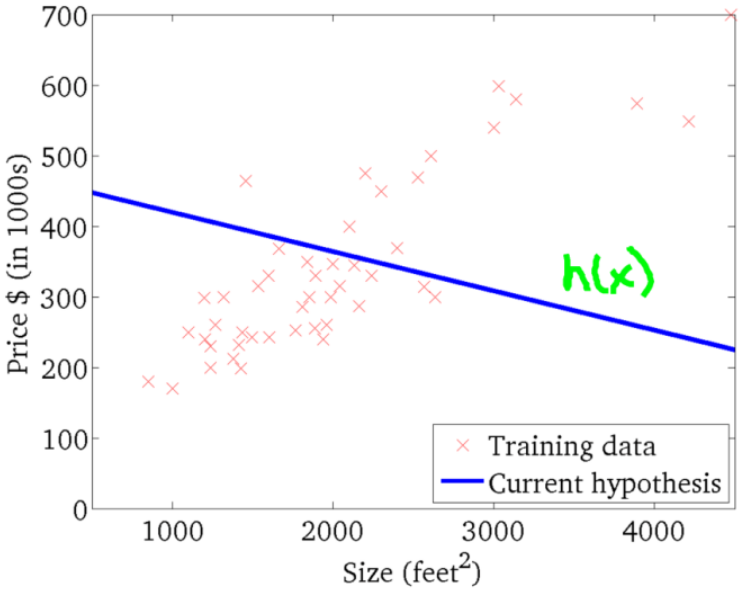
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



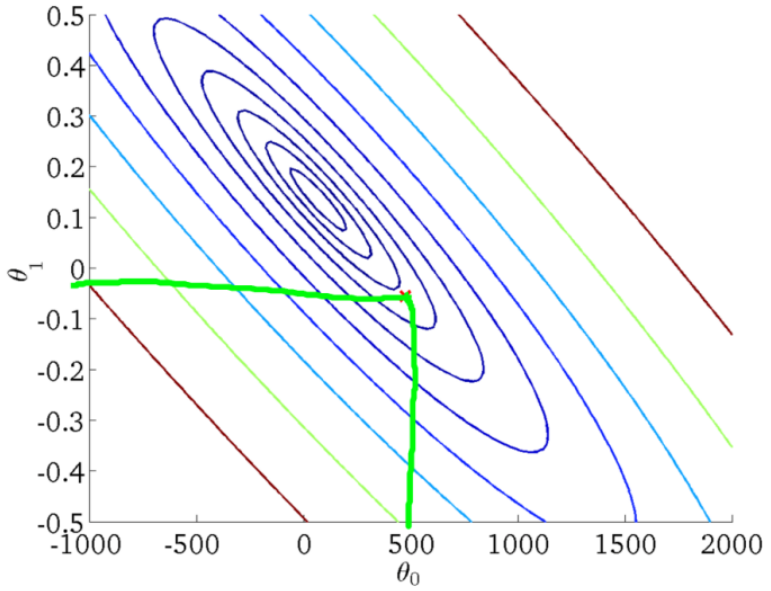
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



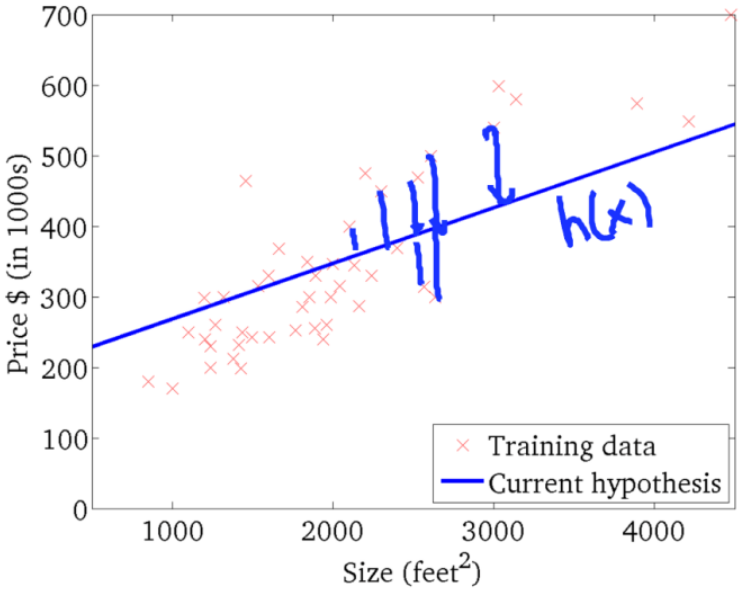
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



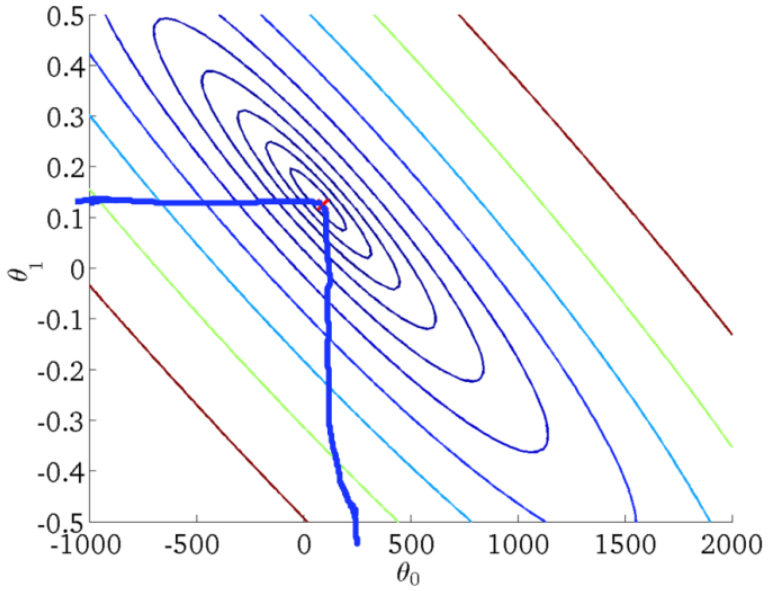
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



Gradient descent

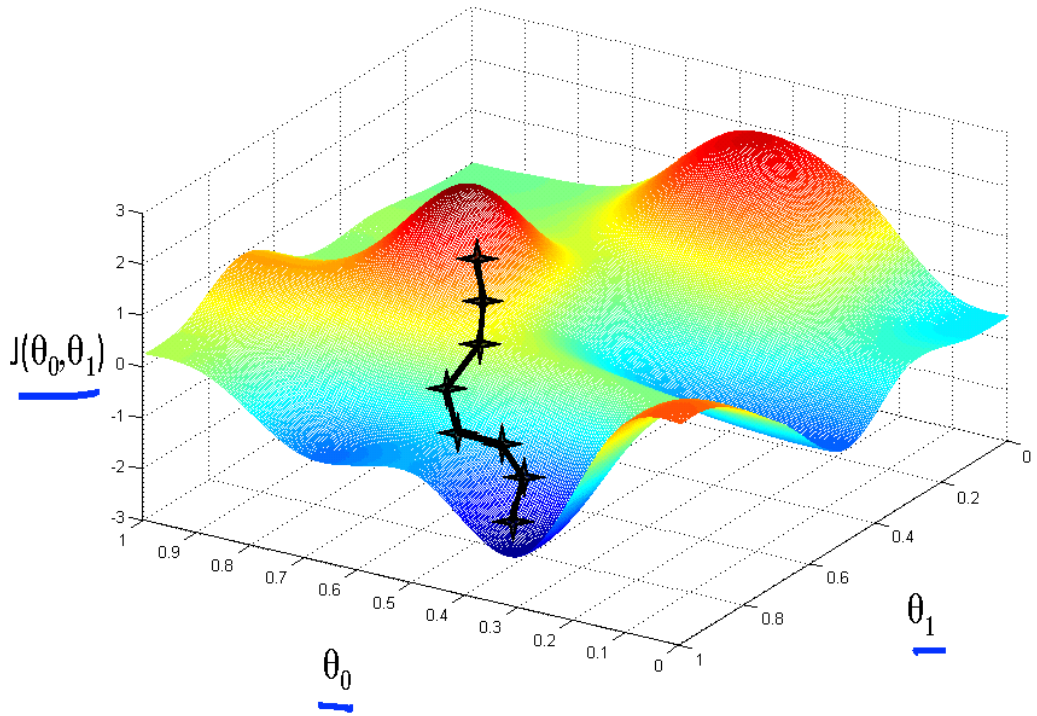
Have some function $J(\theta_0, \theta_1)$ $J(\theta_0, \theta_1, \theta_2, \ldots, \theta_n)$

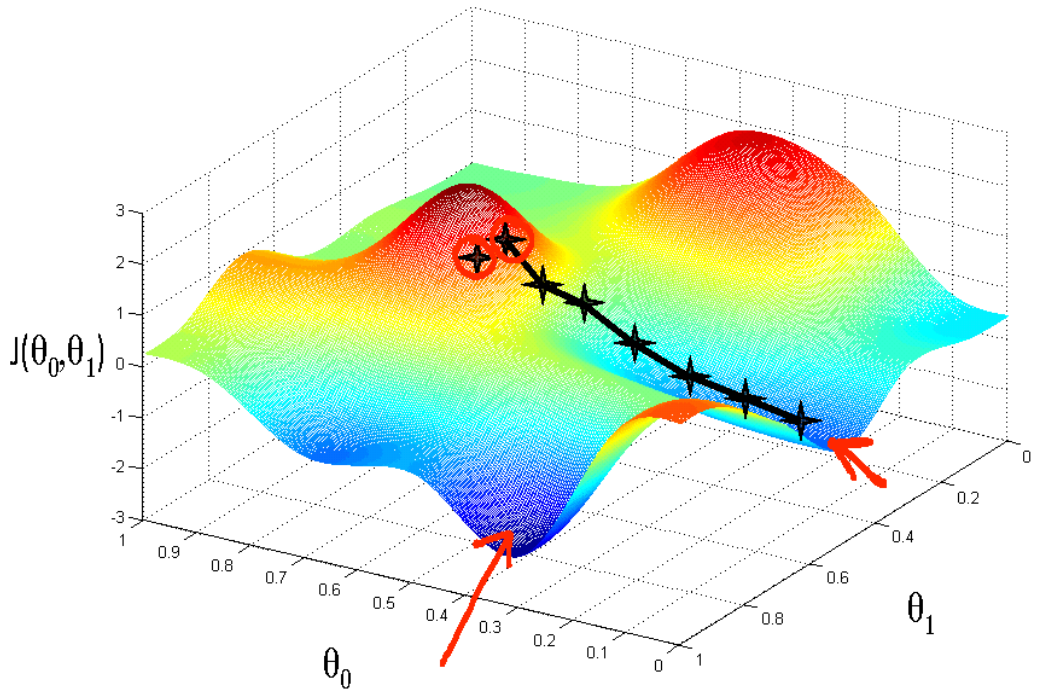
Want $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$ $\min_{\theta_0 \ldots \theta_n} J(\theta_0, \ldots, \theta_n)$

Outline:

- Start with some θ_0, θ_1 (say $\theta_0 = 0, \theta_1 = 0$)
- Keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$

  until we hopefully end up at a minimum


$J(\theta_0,\theta_1)$
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ_0
0
0.2
0.4
0.6
0.8
1
θ_1


J(θ0,θ1)
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1

Gradient descent algorithm

repeat until convergence {

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

} (for $j = 0$ and $j = 1$)

learning rate

Simultaneously update θ_0 and θ_1

Assignment: $a := b$, $a := a + 1$

Truth assertion: $a = b$, $a = a + 1$ ✗

Correct: Simultaneous update

$$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$
$$\theta_0 := \text{temp0}$$
$$\theta_1 := \text{temp1}$$

Incorrect:

$$\text{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$
$$\theta_0 := \text{temp0}$$
$$\text{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$
$$\theta_1 := \text{temp1}$$

Gradient descent algorithm

repeat until convergence {

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

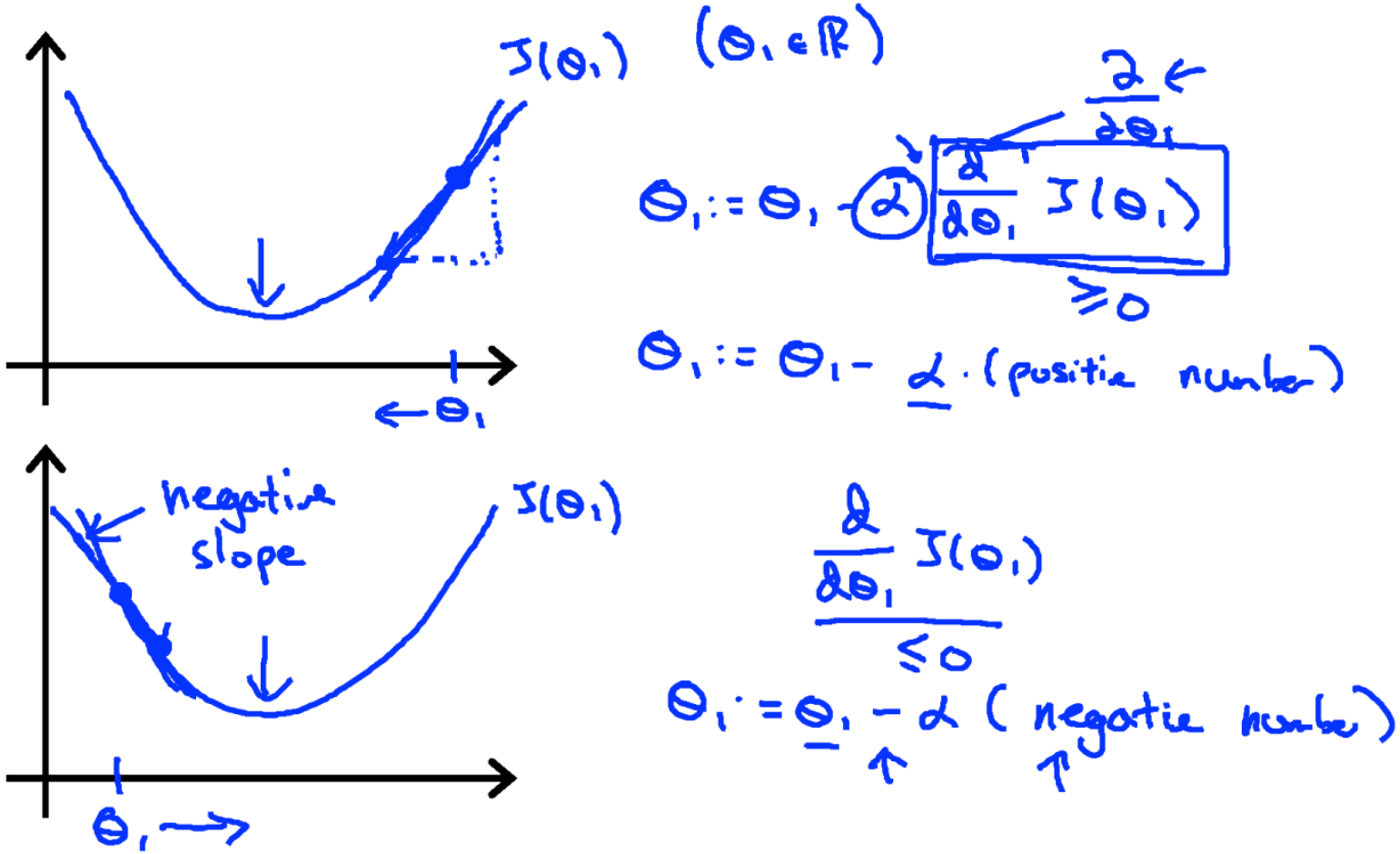
(simultaneously update $j = 0$ and $j = 1$)

}

learning rate

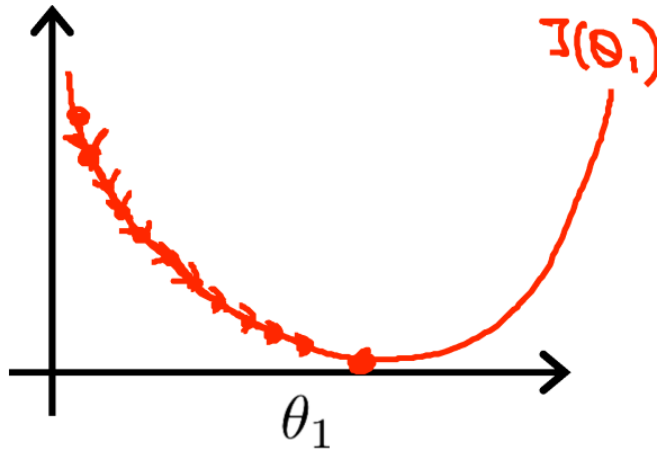
derivative

$\min_{\theta_1} J(\theta_1)$ $\quad \theta_1 \in \mathbb{R}$.

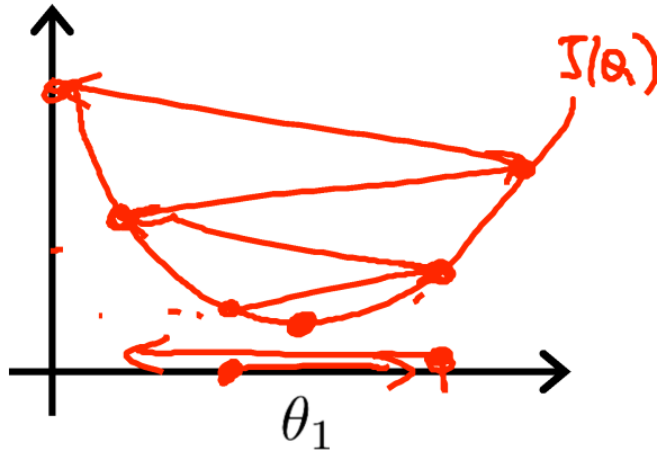

J(θ1)
(θ1 ∈ ℝ)
θ1
negative slope
J(θ1)
θ1
θ1 := θ1 − α (positive number)
θ1 := θ1 − α (negative number)

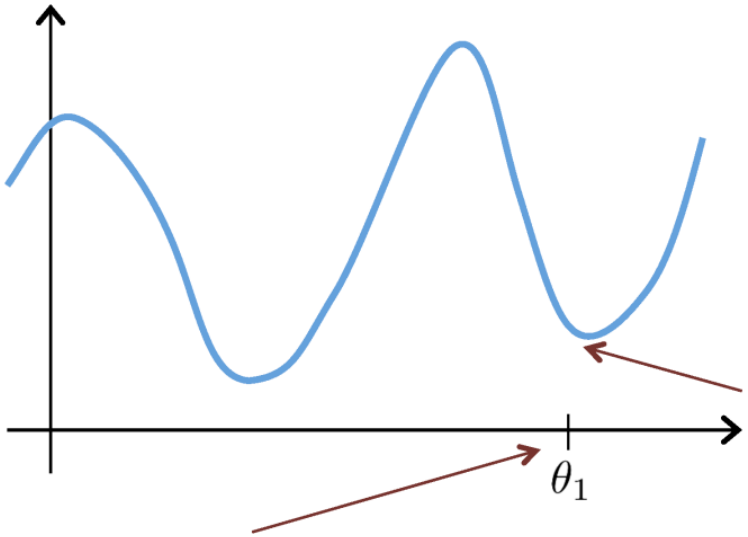
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

If α is too small, gradient descent can be slow.



If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.



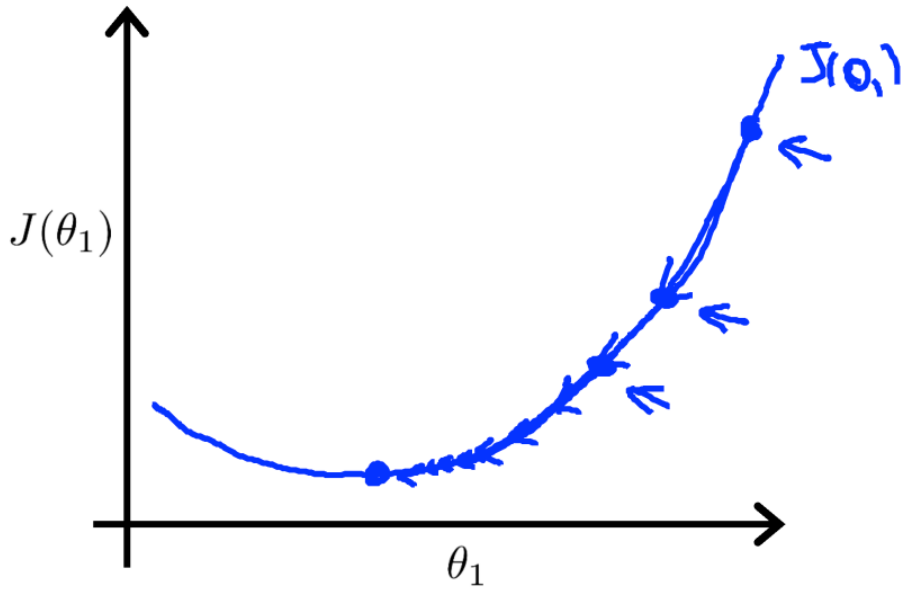


$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

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

$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

As we approach a local minimum, gradient descent will automatically take smaller steps. So, no need to decrease α over time.



Gradient descent algorithm

repeat until convergence {

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

(for $j = 1$ and $j = 0$)

}

Linear Regression Model

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

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

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

$$= \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)^2$$

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

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

Gradient descent algorithm

repeat until convergence {

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

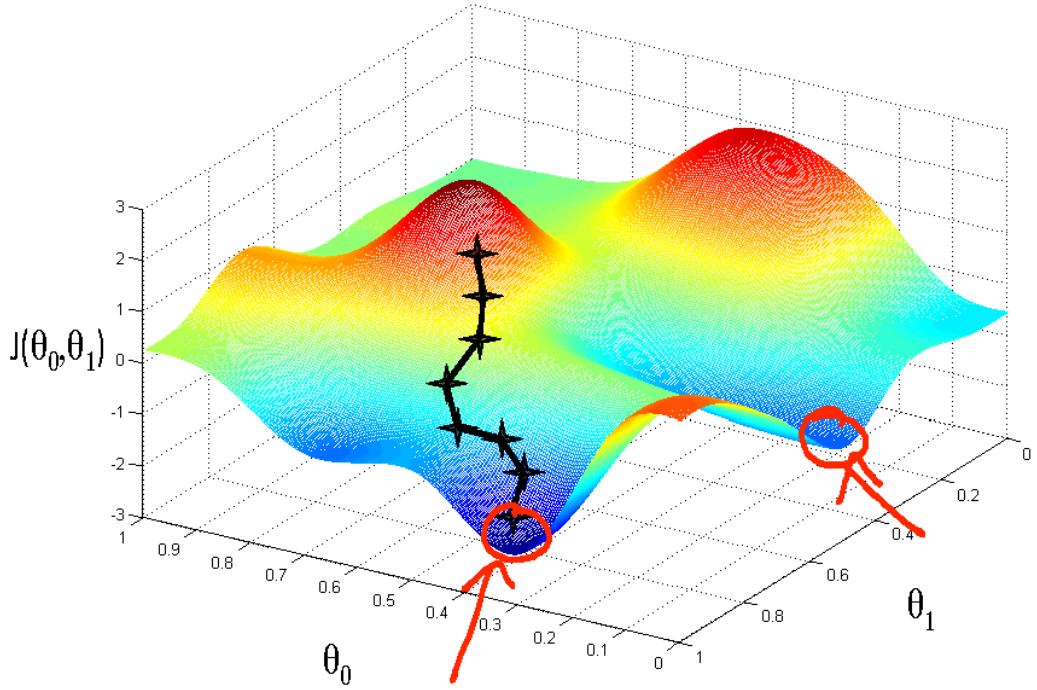
$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x^{(i)}$$

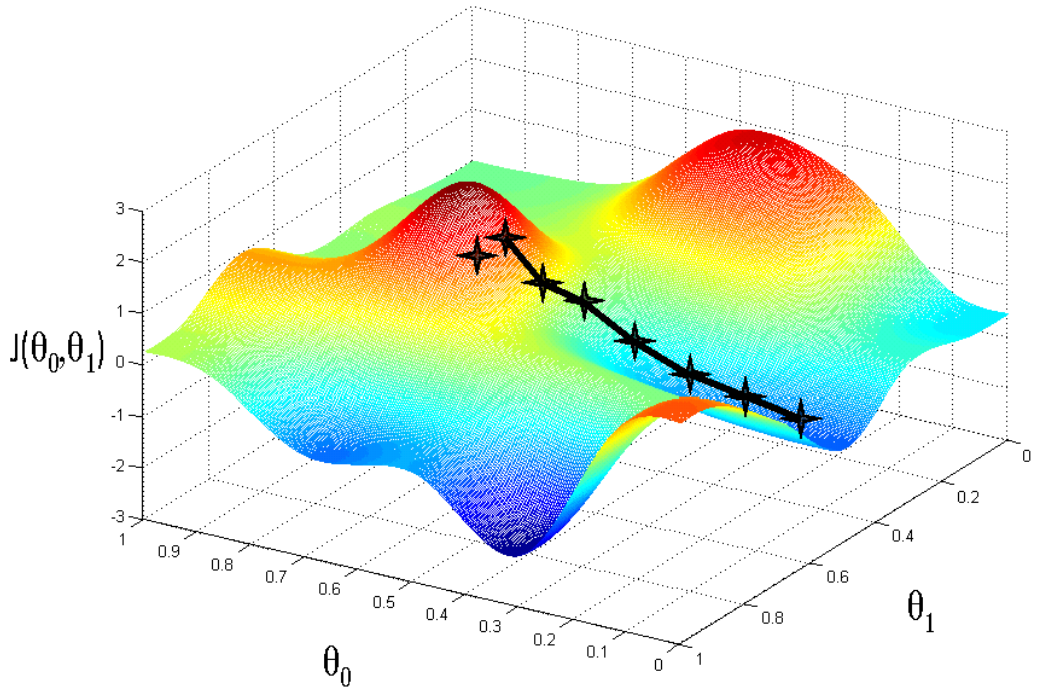
}

$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$

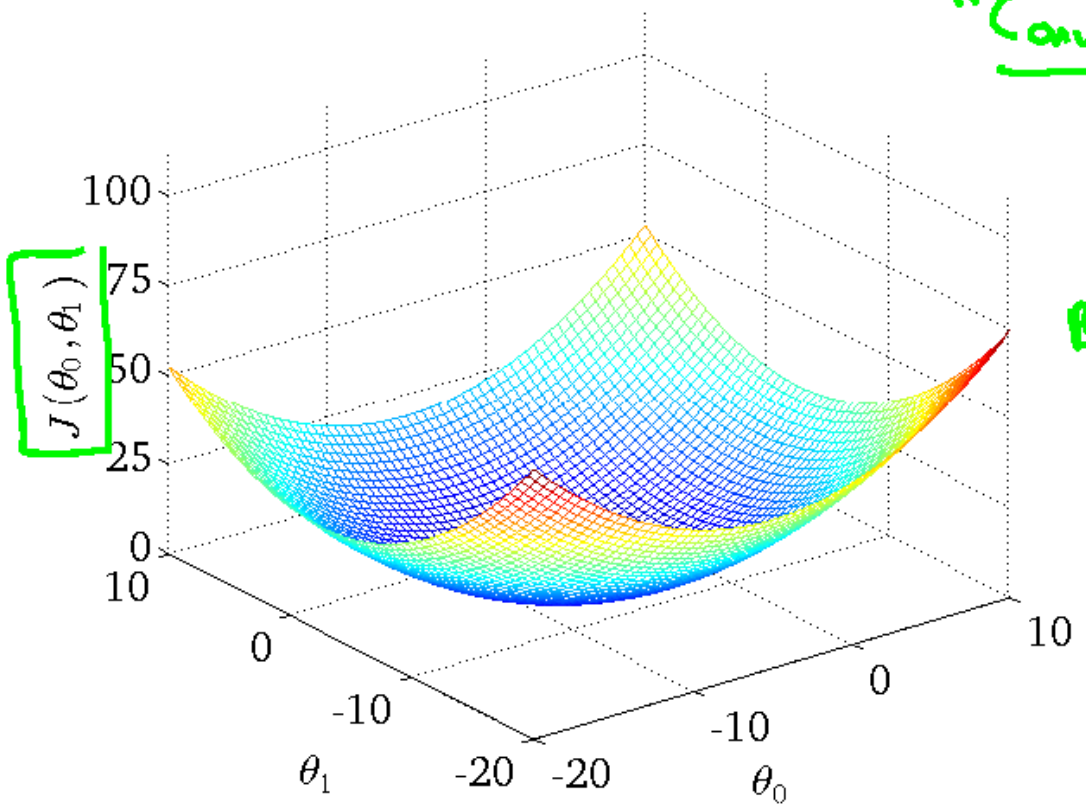
$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$

update θ_0 and θ_1 simultaneously


J(θ0,θ1)
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1


J(θ0,θ1)
3
2
1
0
-1
-2
-3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1

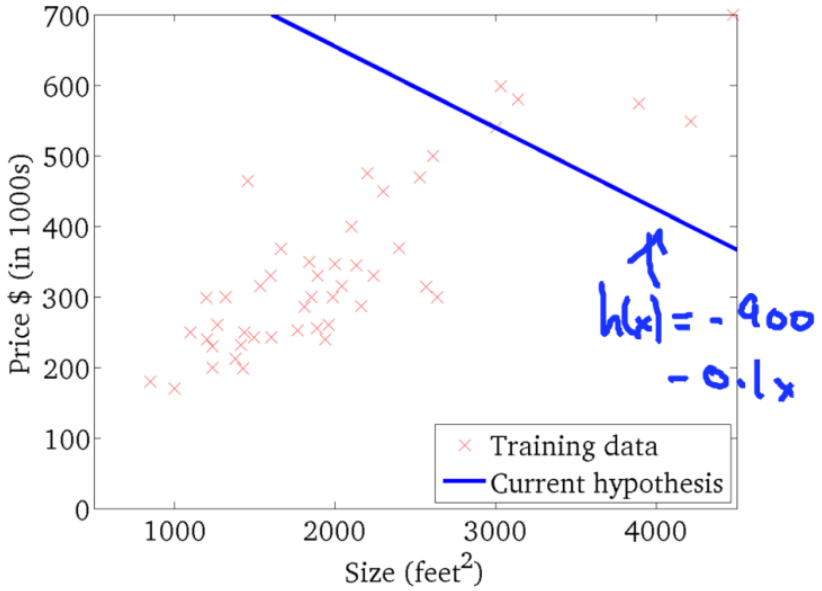
"Convex function"



Bowl-shaped

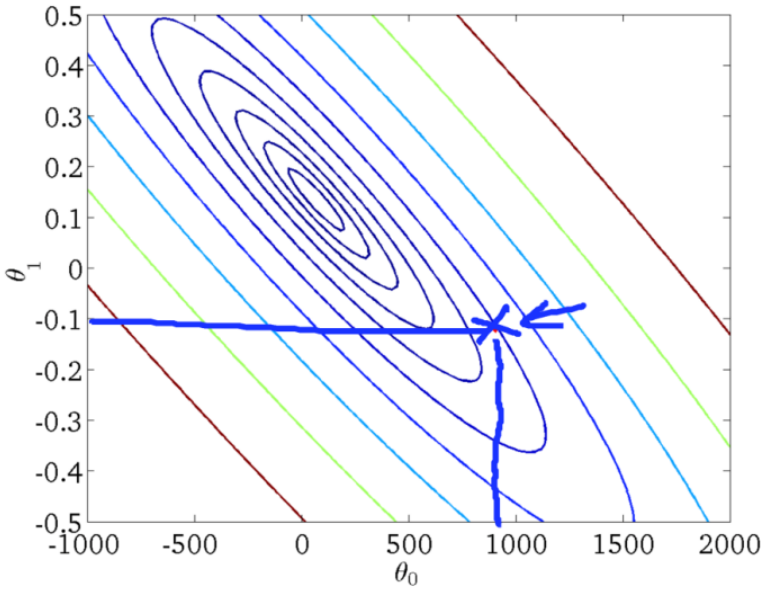
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



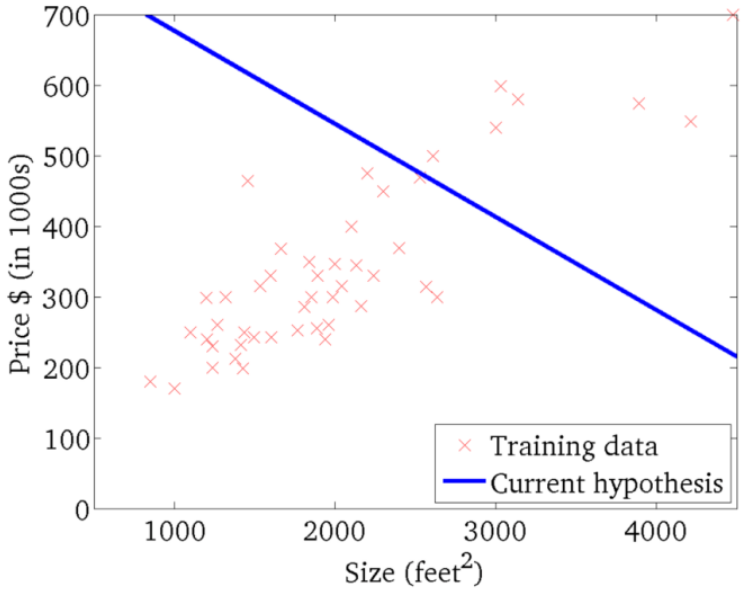
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



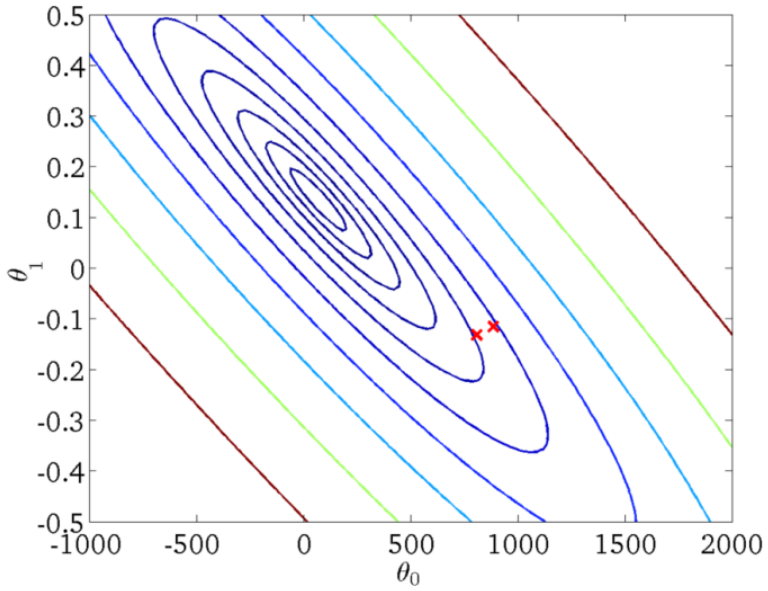
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



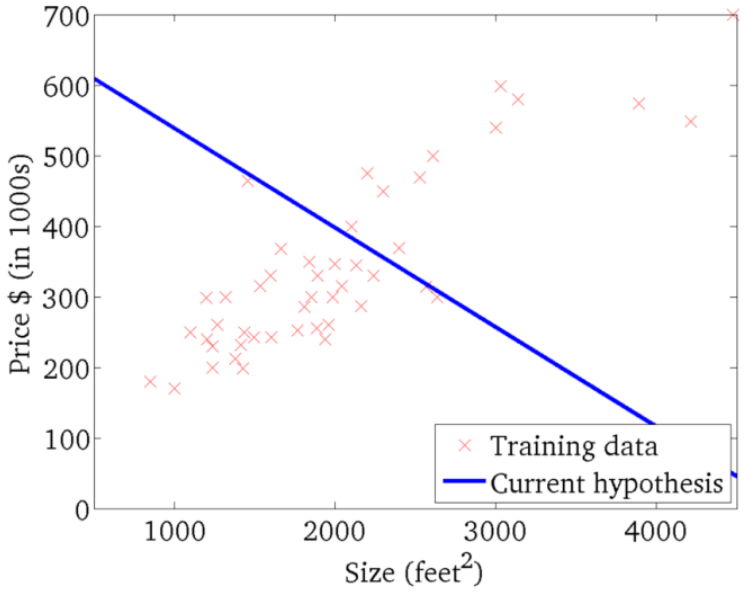
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



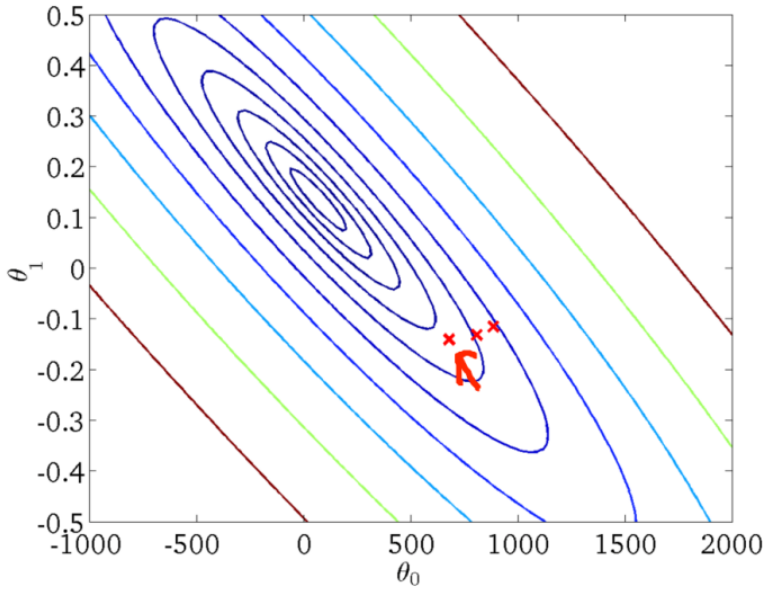
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



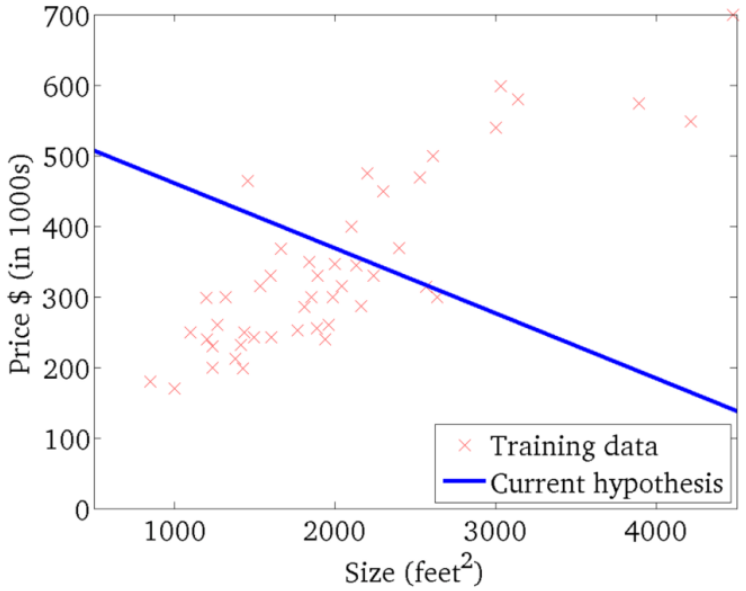
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



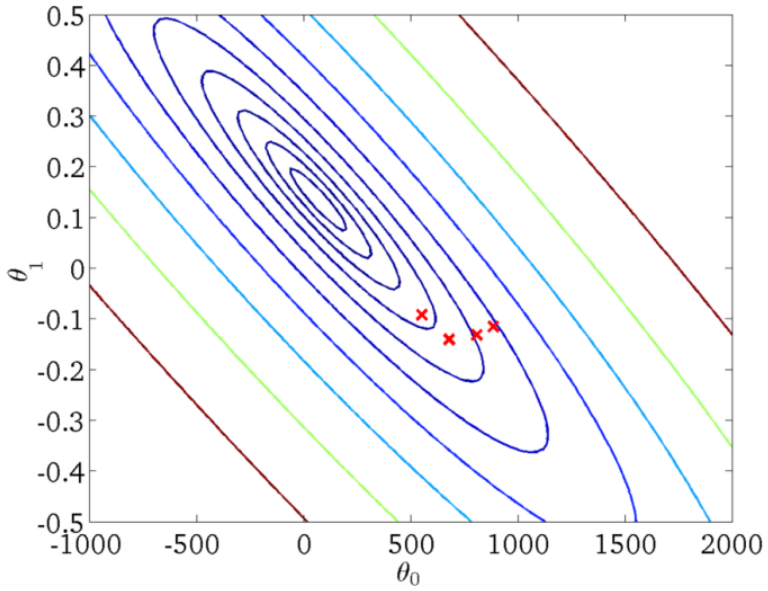
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



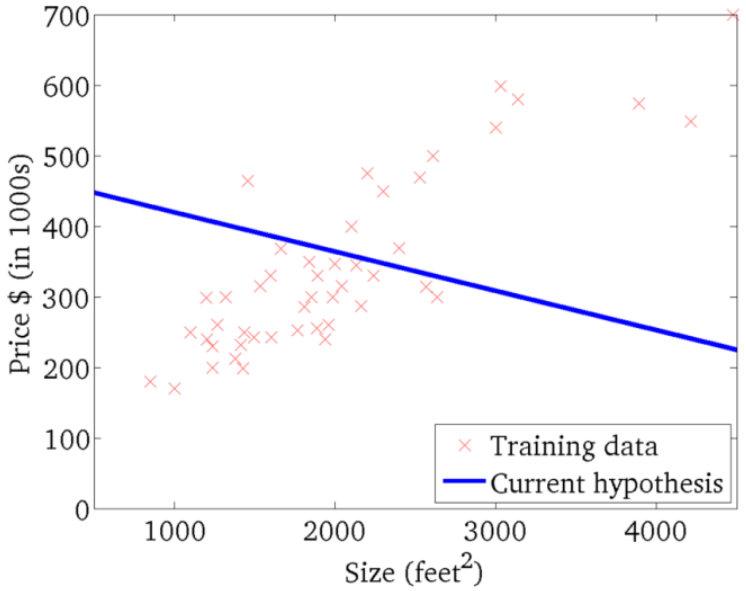
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



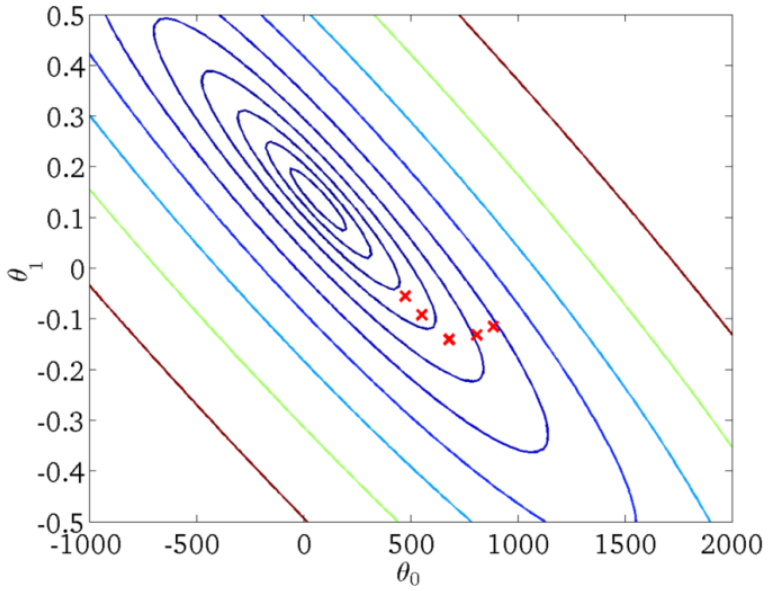
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



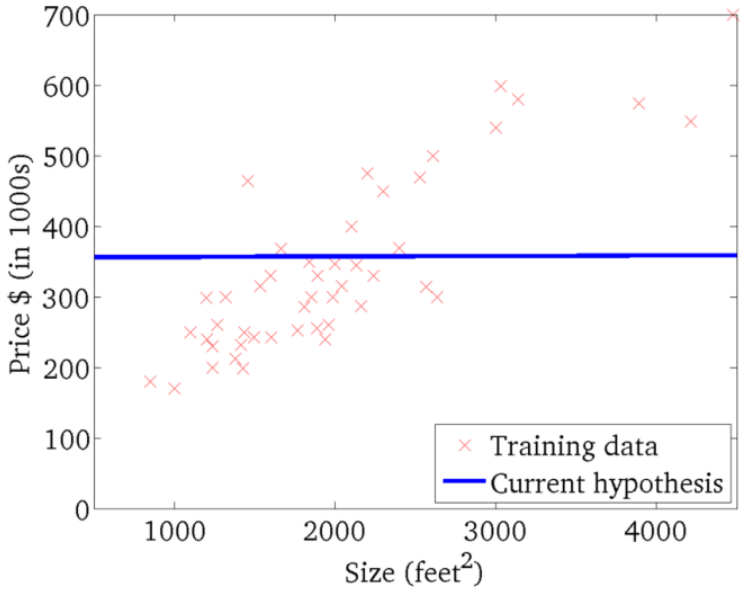
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



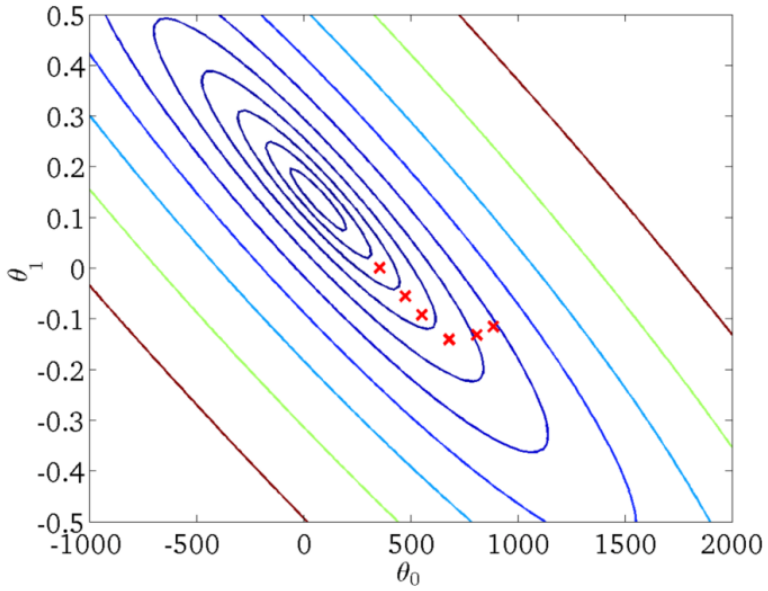
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



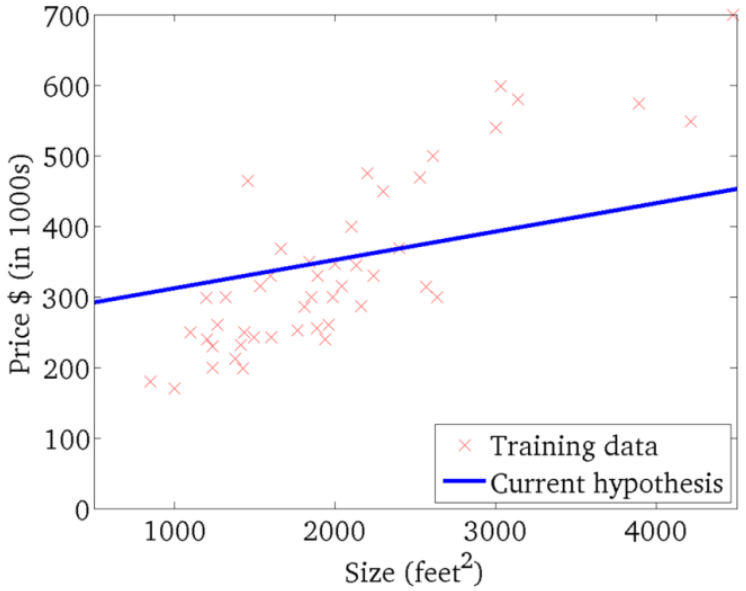
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



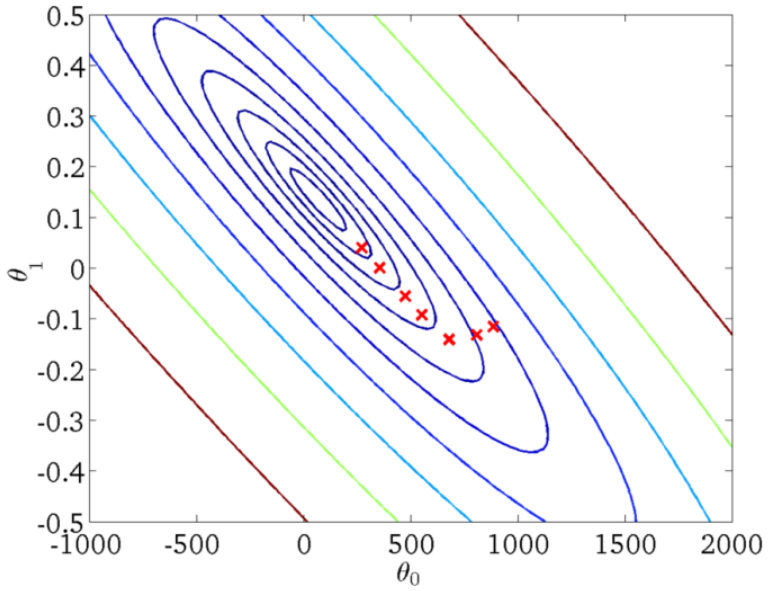
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



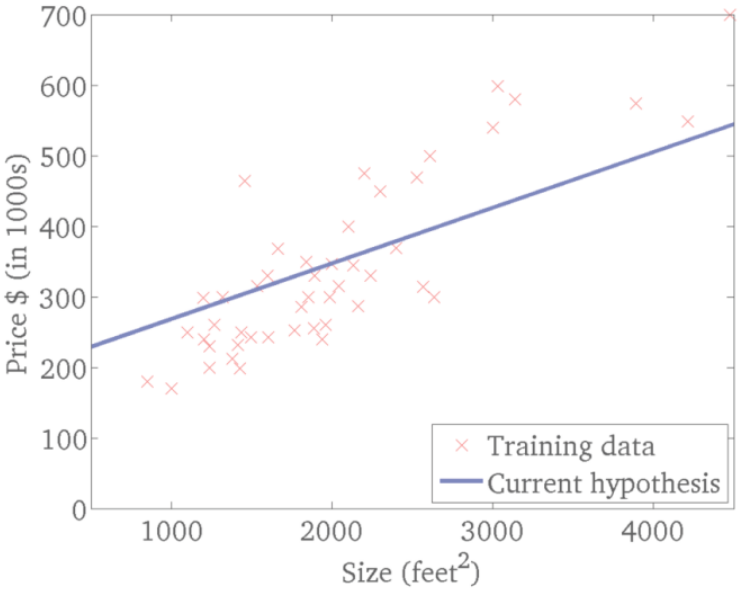
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



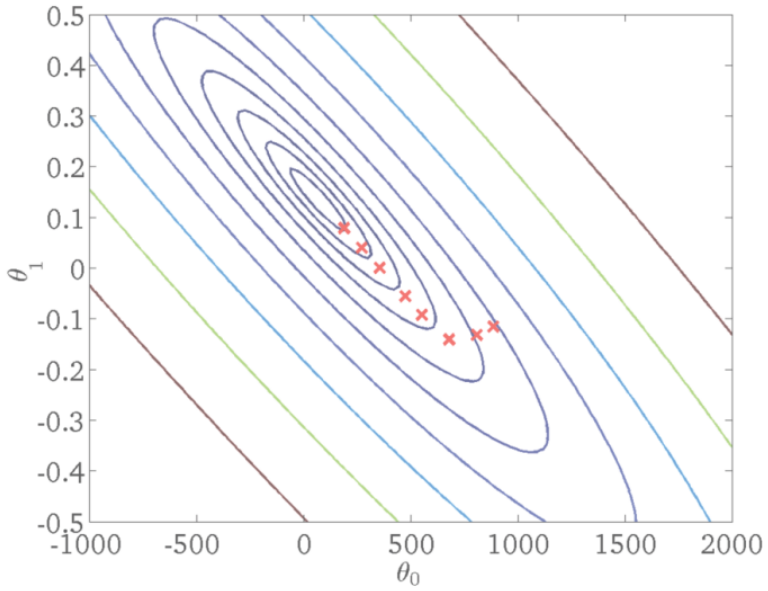
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



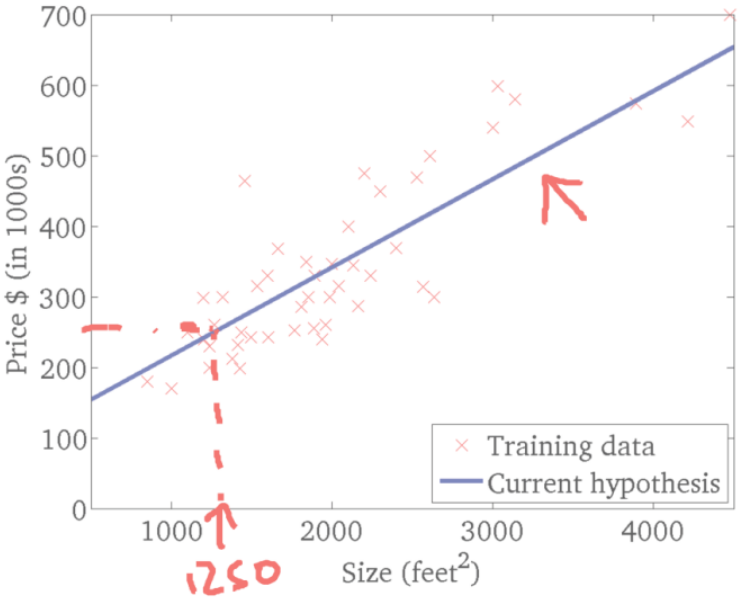
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



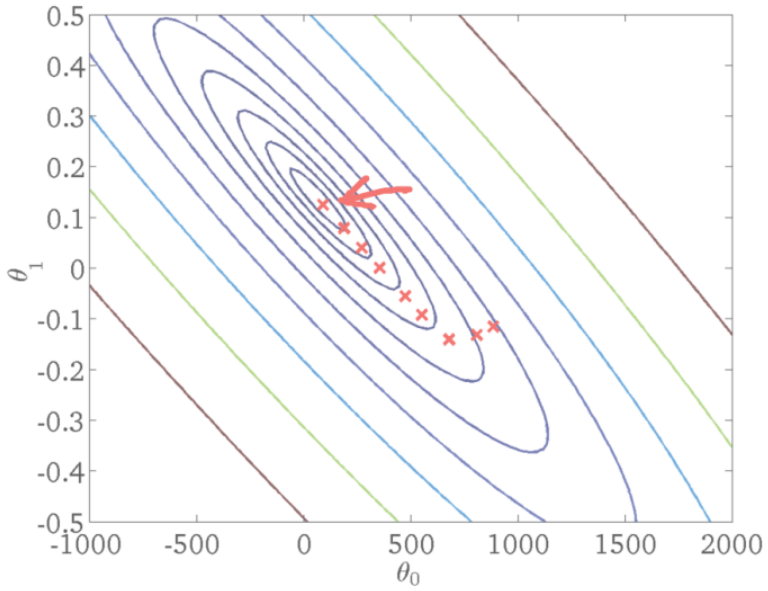
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



"Batch" Gradient Descent

"Batch": Each step of gradient descent uses all the training examples.

$$\sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

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
...	...

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

Multiple features (variables).

Size (feet²) 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
...	...	...	...	...

$m = 47$

$n = 4$

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

$x_3^{(2)} = 2$

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.

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

x_2: blood pressure; x_3: family history; 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 $x_0 = 1$. $(x_0^{(i)} = 1)$

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

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

$$= \theta^T x$$

θ^T: $(n+1) \times 1$ matrix

$\theta^T x$

x

Multivariate linear regression.

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 $\{$

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

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

$\}$

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

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

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

$\ldots$

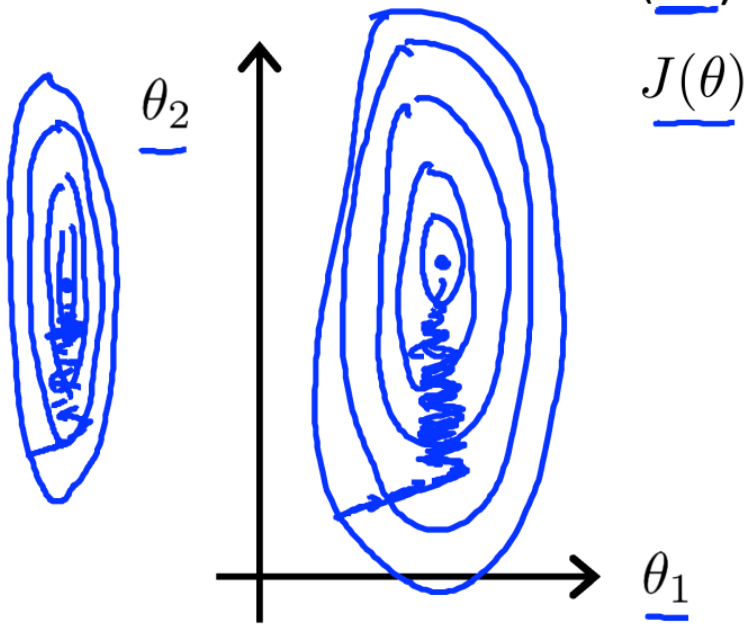
Gradient descent in practice I: Feature Scaling

Feature Scaling

Idea: Make sure features are on a similar scale.

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

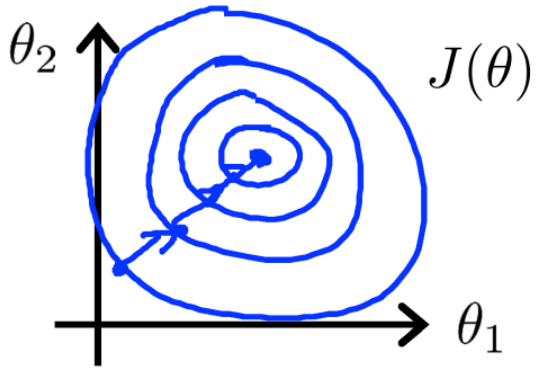
x_2 = number of bedrooms (1-5)



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

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

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



Feature Scaling

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

$x_0 = 1$

$0 \leq x_1 \leq 3$ ✓

$-2 \leq x_2 \leq 0.5$ ✓

$-100 \leq x_3 \leq 100$ ✗

$-0.0001 \leq x_4 \leq 0.0001$ ✗

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

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

Average size = 100

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)

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

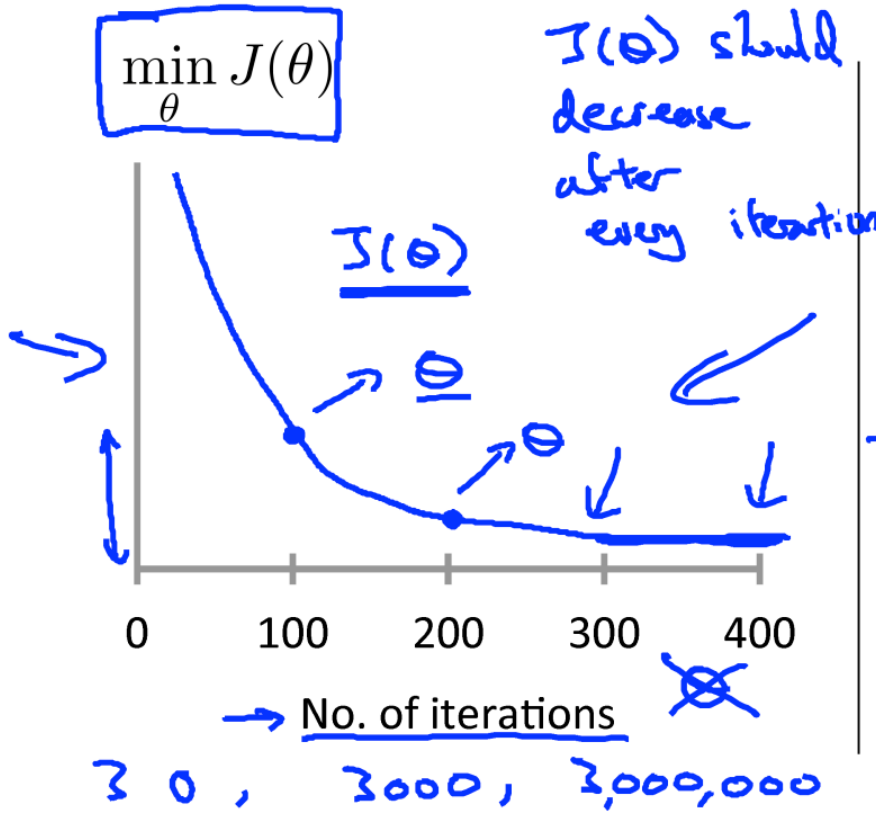
Gradient descent in practice II: Learning rate

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.

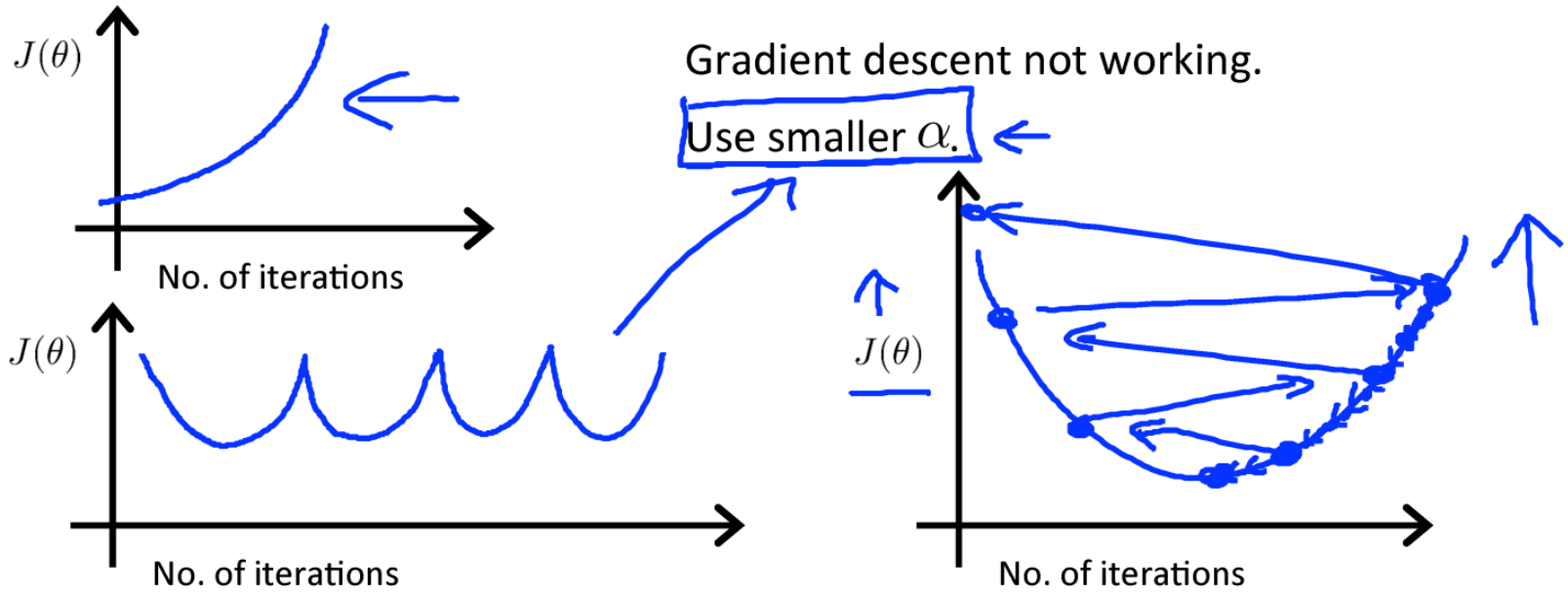


→ Example automatic convergence test:

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

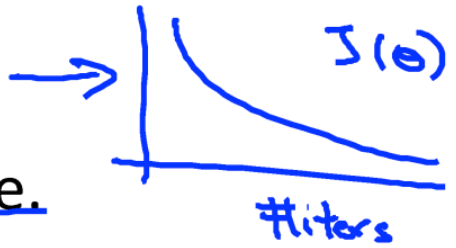
ε

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

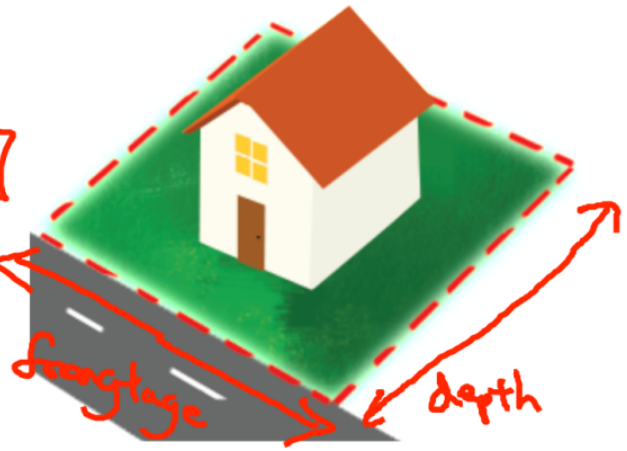
$$\ldots, 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, \ldots$$

Features and polynomial regression

Housing prices prediction

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

x_1 x_2



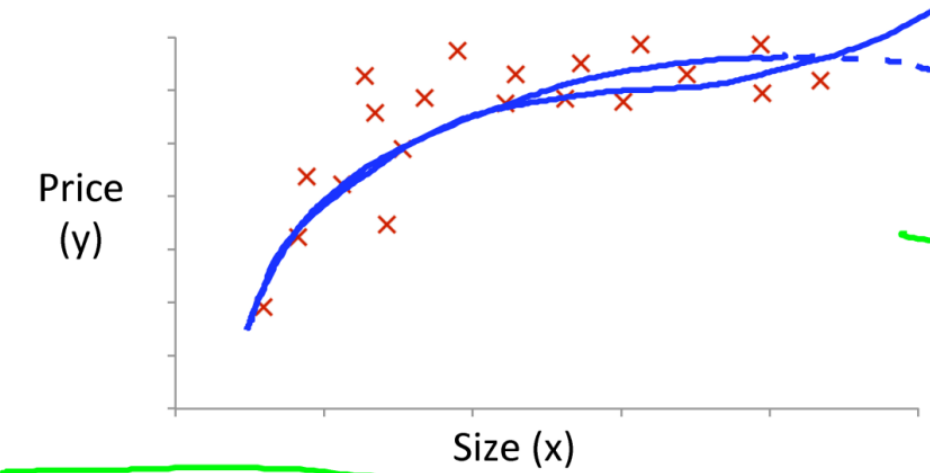
Area

x = frontage * depth

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

↑ land area

Polynomial regression



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

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

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

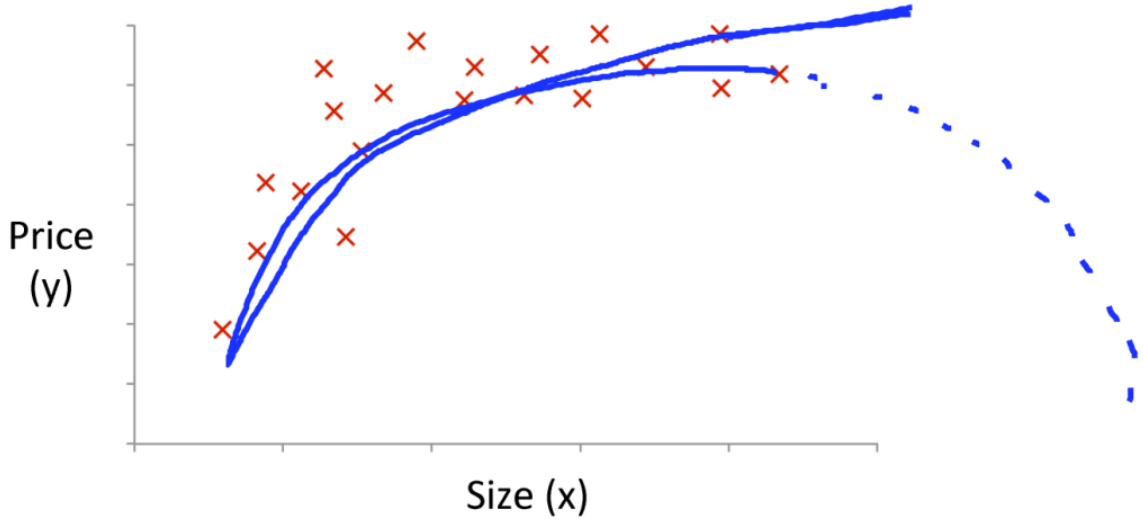
$$x_1 = (size)$$
$$x_2 = (size)^2$$
$$x_3 = (size)^3$$

Size: 1 - 1000

$Size^2$: 1 - 1000,000

$Size^3$: 1 - 10^9

Choice of features

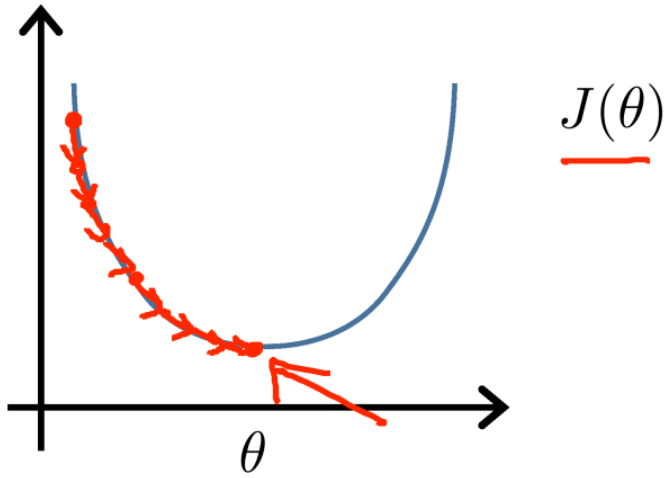


$$h_\theta(x) = \theta_0 + \theta_1(size) + \theta_2(size)^2$$

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

Normal equation

Gradient Descent



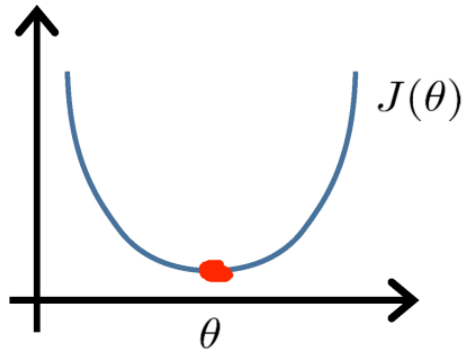
Normal equation: Method to solve for θ analytically.

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

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

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

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

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

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

(design matrix) X =

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

$m \times (n+1)$

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

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

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

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

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

$(X^T X)^{-1}$ 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~~

$0 \le x_1 \le 1$

$0 \le x_2 \le 1000$

$0 \le x_3 \le 10^{-5}$ ✓

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 $(X^T X)^{-1}$
	• Slow if n is very large.

$n = 10^6$

$n \times n$ $O(n^3)$

$n = 100$
$n = 1000$
$n = 10000$

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`

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

$1\,m = 3.28$ feet

$\rightarrow n = 10$

$\rightarrow n = 100$

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

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

Logistic Regression

Classification

Classification

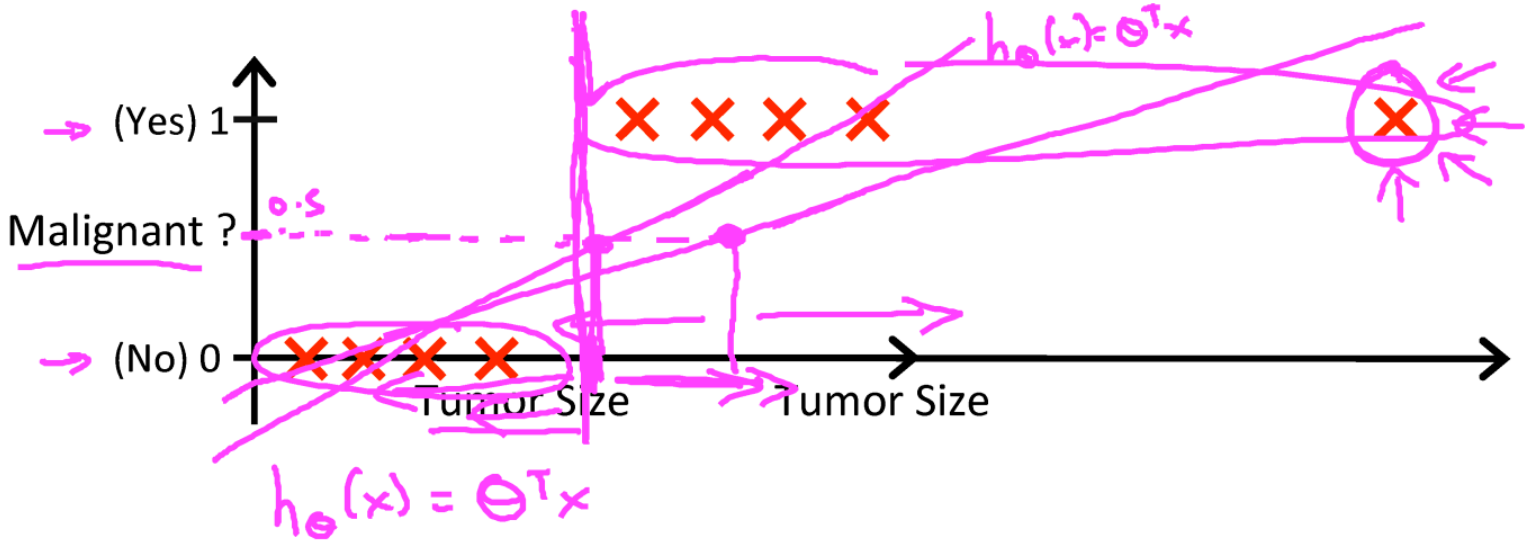
- Email: Spam / Not Spam?
- Online Transactions: Fraudulent (Yes / No)?
- Tumor: Malignant / Benign ?

$y \in \{0, 1\}$

0: "Negative Class" (e.g., benign tumor)

1: "Positive Class" (e.g., malignant tumor)

$y \in \{0, 1, 2, 3\}$



- Threshold classifier output $h_\theta(x)$ at 0.5:
  - If $h_\theta(x) \geq 0.5$, predict "y = 1"
  - If $h_\theta(x) < 0.5$, predict "y = 0"

Classification: y = 0 or 1

$h_\theta(x)$ can be > 1 or < 0

Logistic Regression: $0 \leq h_\theta(x) \leq 1$

Classification

Logistic Regression

Hypothesis Representation

Logistic Regression Model

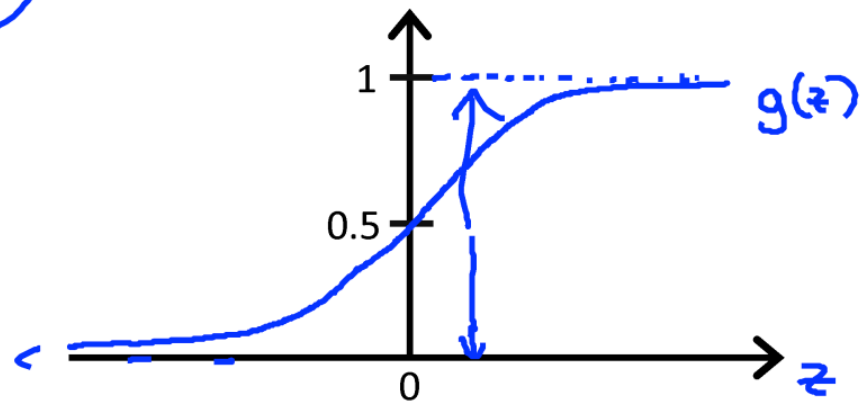
Want $0 \leq h_\theta(x) \leq 1$

$$h_\theta(x) = g(\theta^T x)$$

$$g(z) = \frac{1}{1+e^{-z}}$$

$z = \theta^T x$

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$



Parameters θ.

- Sigmoid function
- Logistic function

Interpretation of Hypothesis Output

$h_\theta(x)$

$h_\theta(x)$ = estimated probability that y = 1 on input x

Example: If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$

$h_\theta(x) = 0.7$ $\quad$ $y=1$

Tell patient that 70% chance of tumor being malignant

$h_\theta(x) = P(y=1|x;\theta)$

$y = 0$ or 1

"probability that y = 1, given x, parameterized by θ"

$P(y=0|x;\theta) + P(y=1|x;\theta) = 1$

$P(y=0|x;\theta) = 1 - P(y=1|x;\theta)$

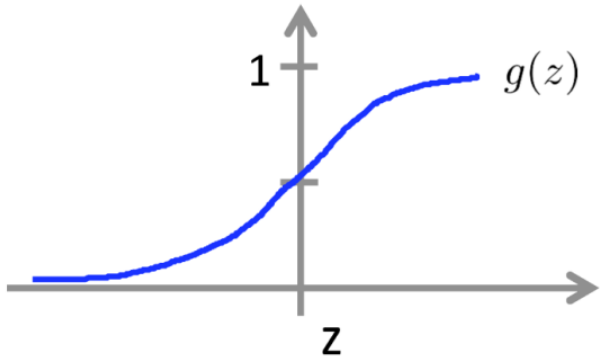
Logistic Regression

Decision boundary

Logistic regression

$$h_\theta(x) = g(\theta^T x)$$

$$g(z) = \frac{1}{1+e^{-z}}$$



Suppose predict "$y = 1$" if $h_\theta(x) \geq 0.5$

$\theta^T x \geq 0$

$g(z) \geq 0.5$ when $z \geq 0$

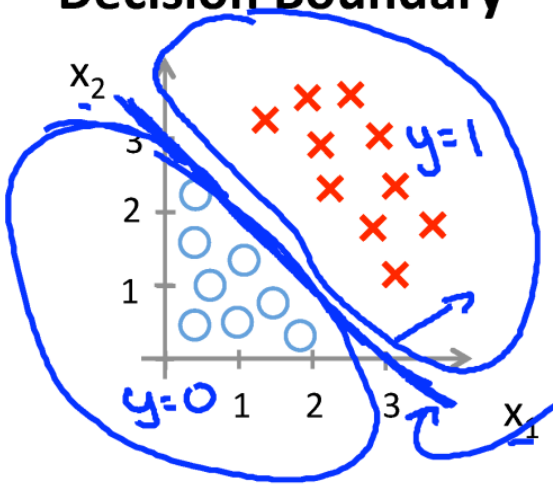
$h_\theta(x) = g(\theta^T x)$

predict "$y = 0$" if $h_\theta(x) < 0.5$

$\theta^T x < 0$

$g(z) < 0.5$ when $z < 0$

Decision Boundary



$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$

$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

-3 1 1

Decision boundary

Predict "$y = 1$" if $-3 + x_1 + x_2 \geq 0$

$\theta^T x$

x_1, x_2

$h_\theta(x) = 0.5$

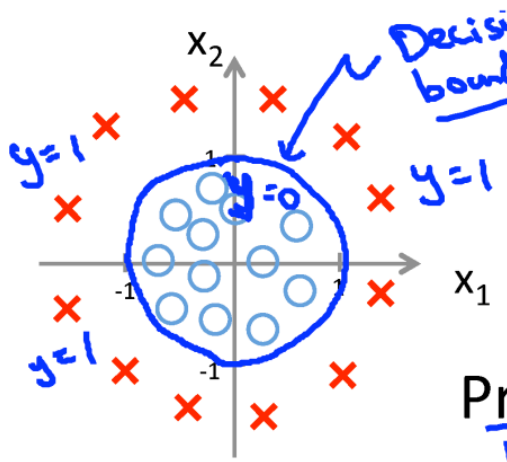
$x_1 + x_2 = 3$

$x_1 + x_2 \geq 3$

$x_1 + x_2 < 3$

$y = 0$

Non-linear decision boundaries



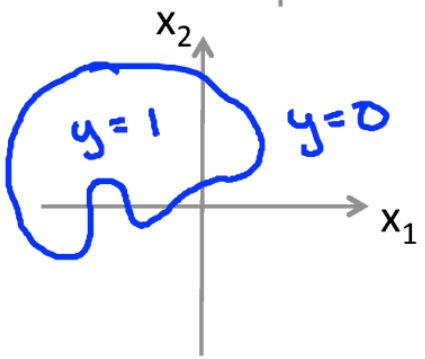
$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$

Predict "$y = 1$" if $-1 + x_1^2 + x_2^2 \geq 0$

$x_1^2 + x_2^2 = 1$

$x_1^2 + x_2^2 \geq 1$



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_1^2 x_2 + \theta_5 x_1^2 x_2^2 + \theta_6 x_1^3 x_2 + \dots)$$

Logistic Regression

Cost function

Training set:

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$$

m examples

$$x \in \begin{bmatrix} x_0 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} \quad x_0 = 1, y \in \{0, 1\}$$

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

How to choose parameters θ ?

Cost function

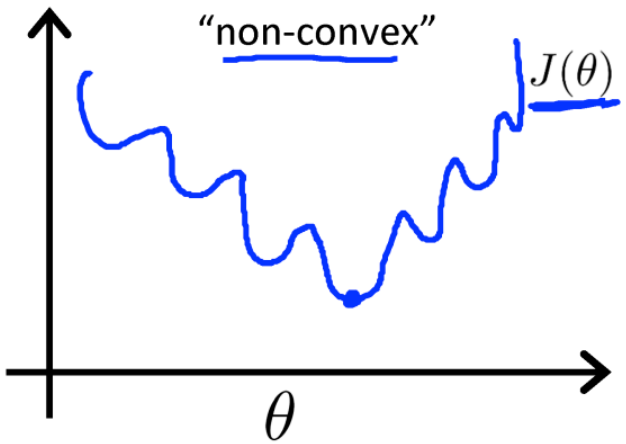
→ ~~Linear~~ regression: $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$

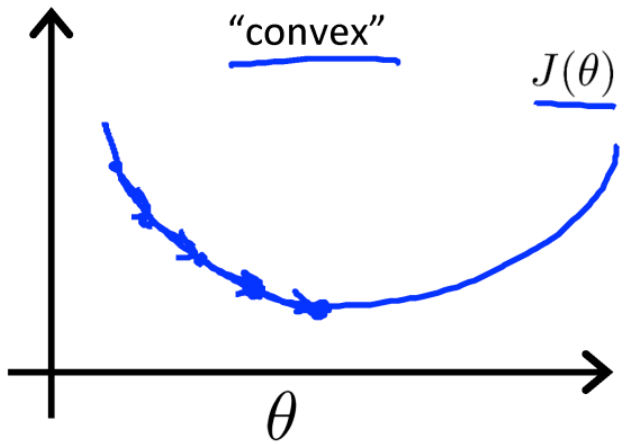
Logistic

$\text{Cost}(h_\theta(x^{(i)}), y^{(i)}) = \frac{1}{2} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$

cost($h_\theta(x^{(i)})$, y)

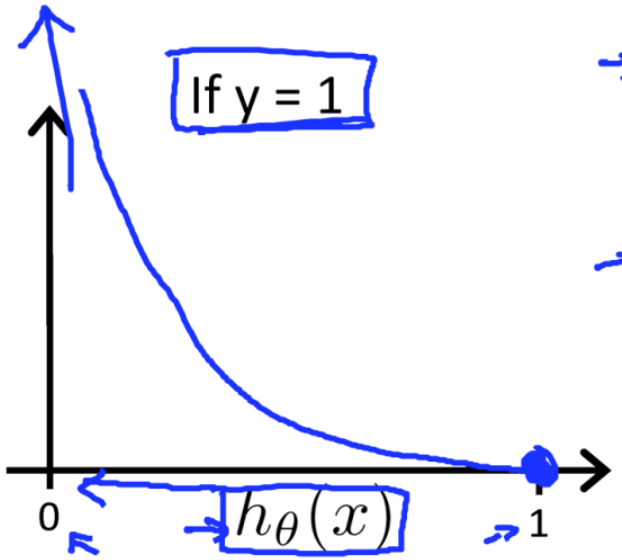
$\frac{1}{1 + e^{-\theta^T x}}$





Logistic regression cost function

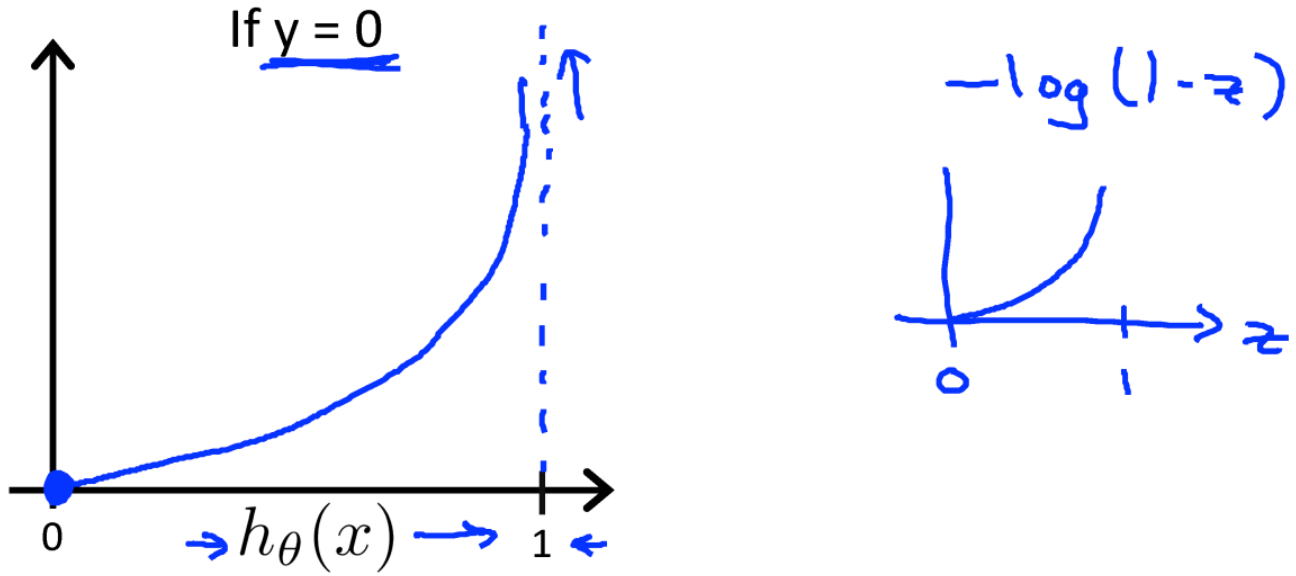
$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$



- $\text{Cost} = 0$ if $y = 1, h_\theta(x) = 1$
  But as $h_\theta(x) \to 0$
  $Cost \to \infty$
- Captures intuition that if $h_\theta(x) = 0$, (predict $P(y = 1|x; \theta) = 0$), but $y = 1$, we'll penalize learning algorithm by a very large cost.

Logistic regression cost function

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$



Logistic Regression

Simplified cost function and gradient decent

Logistic regression cost function

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note: $y = 0$ or 1 always

$$\text{Cost}(h_\theta(x), y) = -y \log(h_\theta(x)) - (1-y) \log(1 - h_\theta(x))$$

If $y = 1$: $\text{Cost}(h_\theta(x), y) = -\log h_\theta(x)$

If $y = 0$: $\text{Cost}(h_\theta(x), y) = -\log(1 - h_\theta(x))$

Logistic regression cost function

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$$

$$= -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

To fit parameters θ :

$$\min_\theta J(\theta)$$ Get θ

To make a prediction given new x:

Output $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$ $p(y=1 \mid x;\theta)$

Gradient Descent

$$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

Want $\min_\theta J(\theta)$:

Repeat $\{$

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

(simultaneously update all θ_j)

$\}$

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

Gradient Descent

$$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

Want $\min_\theta J(\theta)$:

Repeat $\{$

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

(simultaneously update all θ_j)

$\}$

$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$ for $i = 0$ to n

$h_\theta(x) = \theta^T x$

$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$

Algorithm looks identical to linear regression!

Logistic Regression

Advanced optimization

Optimization algorithm

Cost function $J(\theta)$. Want $\min_\theta J(\theta)$.

Given θ, we have code that can compute

- $J(\theta)$
- $\frac{\partial}{\partial \theta_j} J(\theta)$ (for $j = 0, 1, \ldots, n$)

Gradient descent:

Repeat $\{$

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

$\}$

Optimization algorithm

Given θ, we have code that can compute

- $J(\theta)$
- $\frac{\partial}{\partial \theta_j} J(\theta)$ (for $j = 0, 1, \ldots, n$)

Optimization algorithms:

- Gradient descent
- Conjugate gradient
- BFGS
- L-BFGS

Advantages:

- No need to manually pick α
- Often faster than gradient descent.

Disadvantages:

- More complex

Example: $\min_\theta J(\theta)$

$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$ $\theta_1 = 5, \theta_2 = 5.$

$J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$

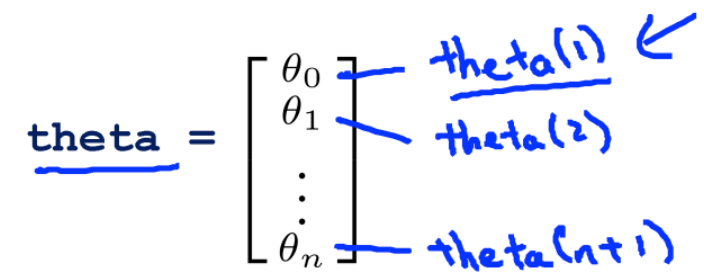
$\frac{\partial}{\partial \theta_1} J(\theta) = 2(\theta_1 - 5)$

$\frac{\partial}{\partial \theta_2} J(\theta) = 2(\theta_2 - 5)$

```
function [jVal, gradient]
            = costFunction(theta)
  jVal = (theta(1)-5)^2 + ...
          (theta(2)-5)^2;
  gradient = zeros(2,1);
  gradient(1) = 2*(theta(1)-5);
  gradient(2) = 2*(theta(2)-5);
```

```
options = optimset('GradObj', 'on', 'MaxIter', '100');
initialTheta = zeros(2,1);
[optTheta, functionVal, exitFlag] ...
    = fminunc(@costFunction, initialTheta, options);
```

$\theta \in \mathbb{R}^d \quad d \geq 2.$



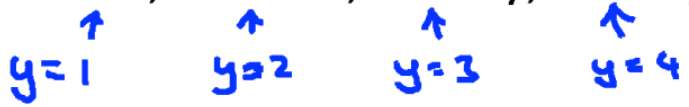

```
function [jVal, gradient] = costFunction(theta)
    jVal = [code to compute J(theta)];
    gradient(1) = [code to compute ∂/∂θ0 J(θ)];
    gradient(2) = [code to compute ∂/∂θ1 J(θ)];
    ⋮
    gradient(n+1) = [code to compute ∂/∂θn J(θ)];
```

Logistic Regression

Multi-class classification: One-vs-all

Multiclass classification

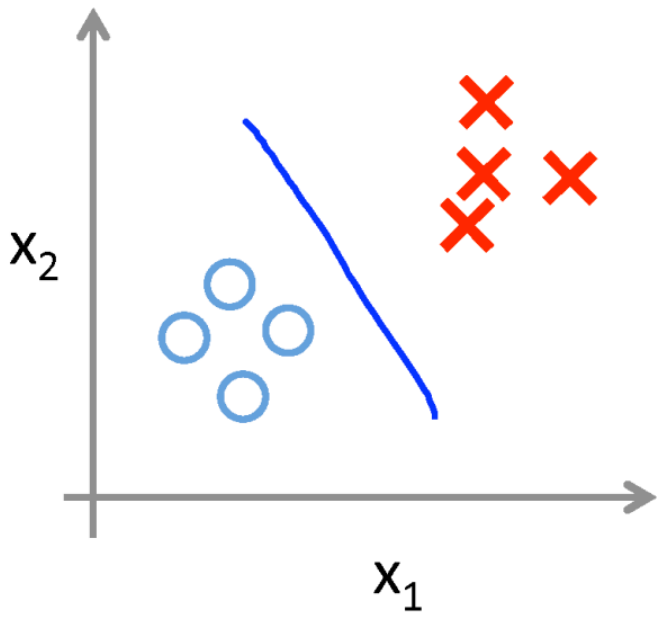
Email foldering/tagging: Work, Friends, Family, Hobby



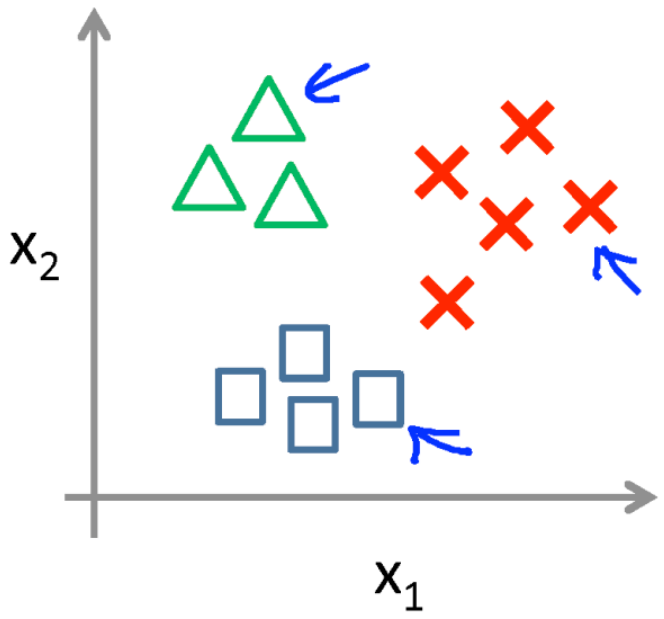
Medical diagrams: Not ill, Cold, Flu

Weather: Sunny, Cloudy, Rain, Snow

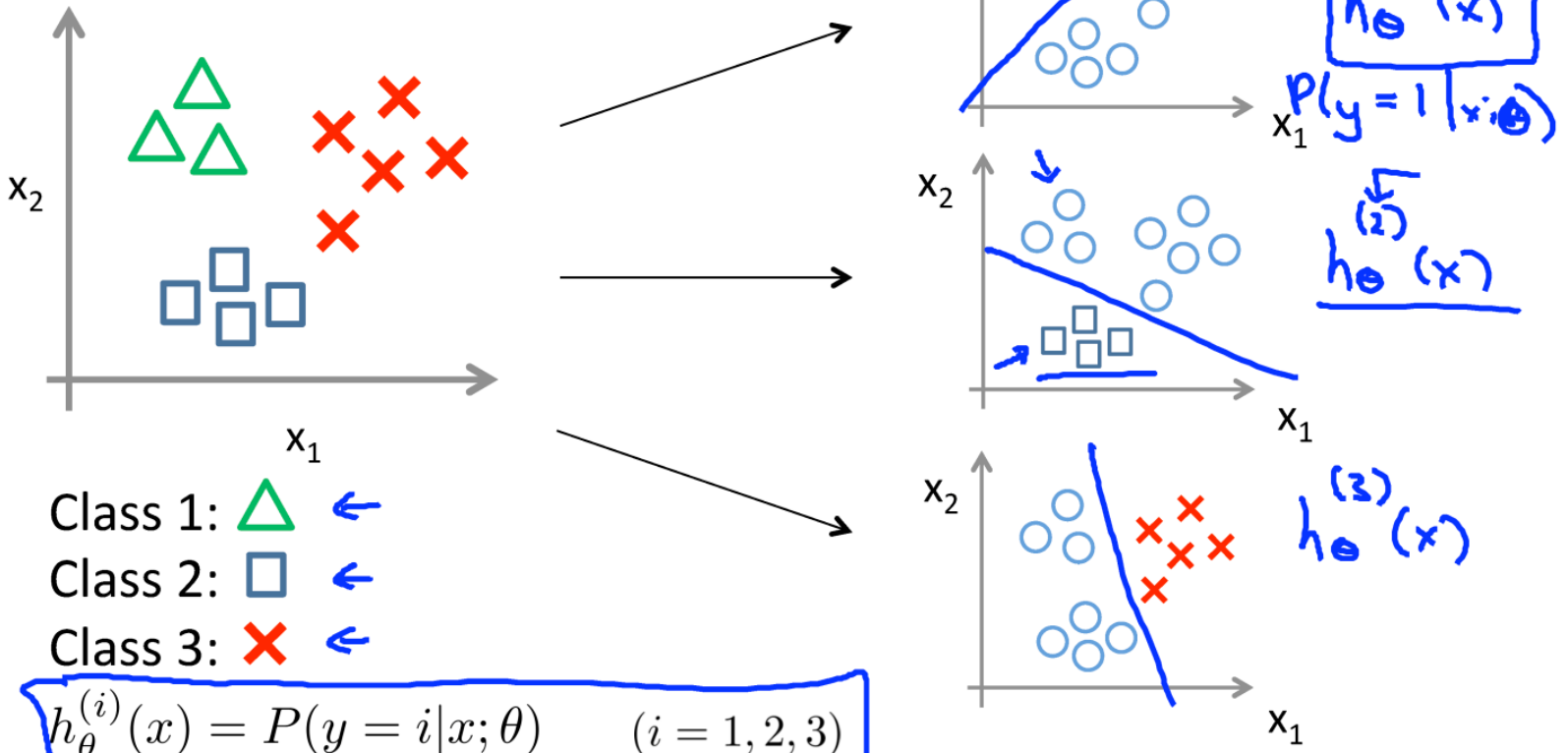
Binary classification:



Multi-class classification:



One-vs-all (one-vs-rest):



One-vs-all

Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i to predict the probability that $y = i$.

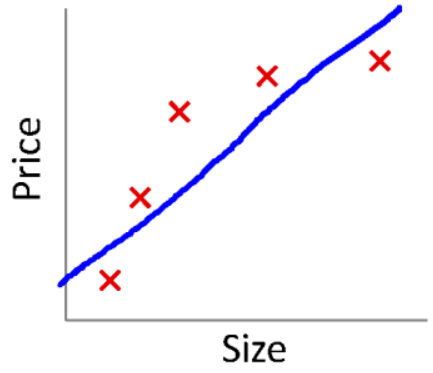
On a new input x, to make a prediction, pick the class i that maximizes

$$\max_i h_\theta^{(i)}(x)$$

Regularization

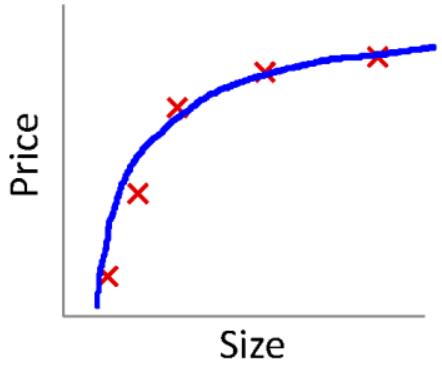
The problem of overfitting

Example: Linear regression (housing prices)



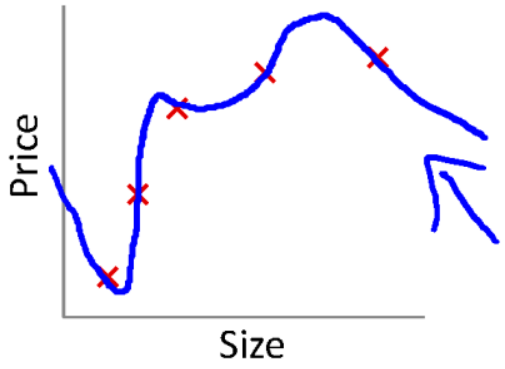
$\rightarrow \theta_0 + \theta_1 x$

"Underfit" "High bias"



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

"Just right"

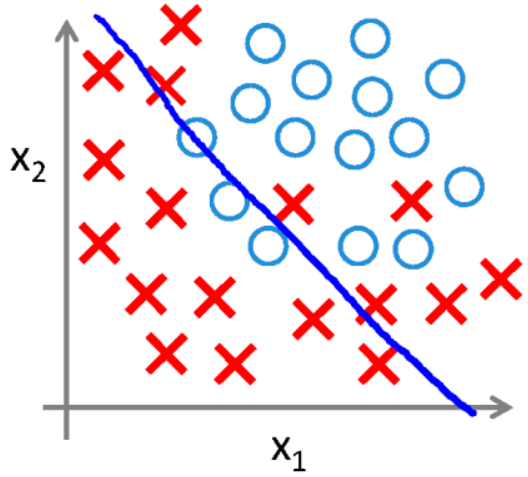


$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

"Overfit" "High variance"

Overfitting: If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

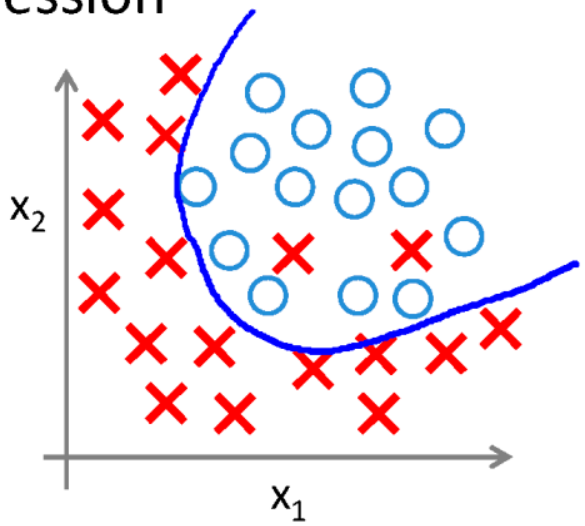
Example: Logistic regression



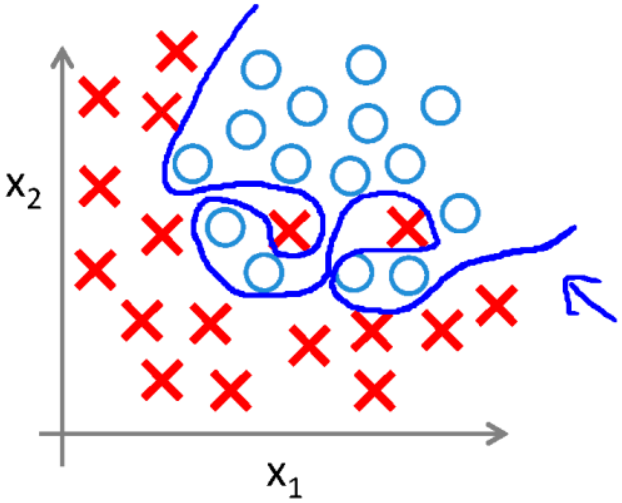
$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

(g = sigmoid function)

"Underfit"



$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2)$

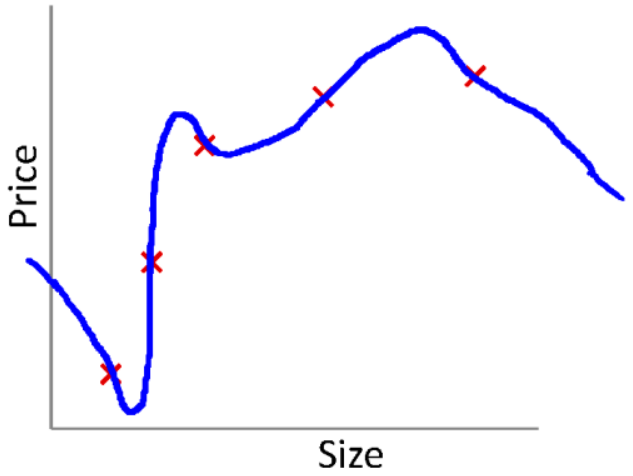


$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

"Overfit"

Addressing overfitting:

$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size
$\vdots$
x_{100}



Addressing overfitting:

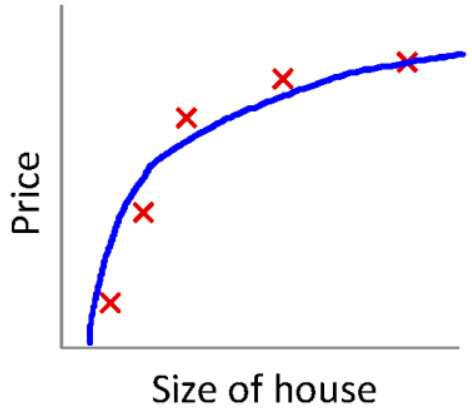
Options:

1. Reduce number of features.
   - — Manually select which features to keep.
   - — Model selection algorithm (later in course).
2. Regularization.
   - — Keep all the features, but reduce magnitude/values of parameters θ_j.
   - — Works well when we have a lot of features, each of which contributes a bit to predicting y.

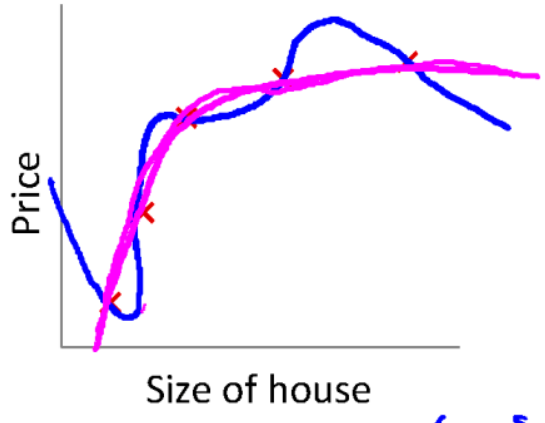
Regularization

Cost function

Intuition



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



$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Suppose we penalize and make θ_3, θ_4 really small.

$$\min_\theta \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\,\theta_3^2 + 1000\,\theta_4^2$$

$\theta_3 \approx 0 \qquad \theta_4 \approx 0$

Regularization.

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$

- "Simpler" hypothesis
- Less prone to overfitting

Housing:

- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

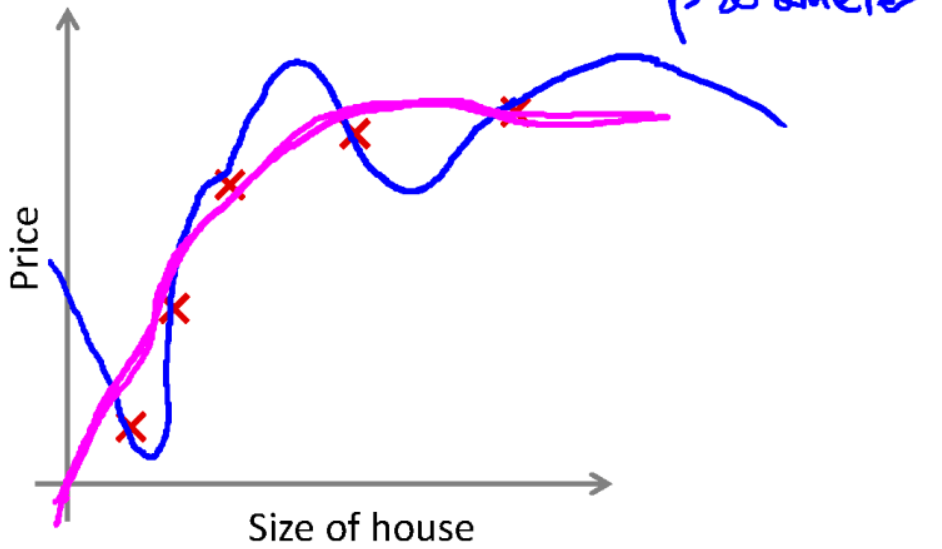
$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

Regularization.

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}\theta_j^2\right]$$

regularization parameter

$$\min_\theta J(\theta)$$



In regularized linear regression, we choose θ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{n}\theta_j^2\right]$$

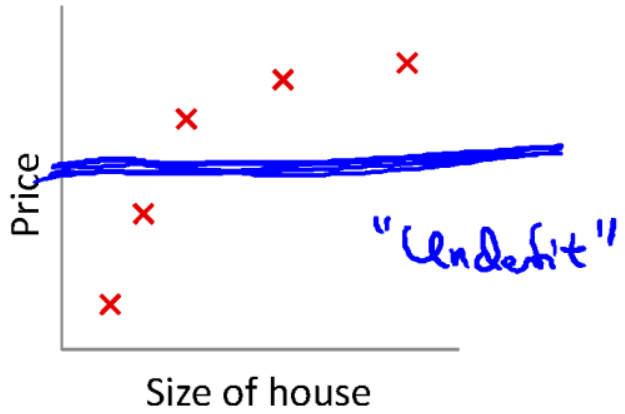
What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?

- Algorithm works fine; setting λ to be very large can't hurt it
- Algortihm fails to eliminate overfitting.
- Algorithm results in underfitting. (Fails to fit even training data well).
- Gradient descent will fail to converge.

In regularized linear regression, we choose θ to minimize

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}\theta_j^2\right]$$

What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?



$h_\theta(x)$

$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

$\theta_1, \theta_2, \theta_3, \theta_4$

$\theta_1 \approx 0, \theta_2 \approx 0$

$\theta_3 \approx 0, \theta_4 \approx 0$

$h_\theta(x) = \theta_0$

Regularization

Regularized linear regression

Regularized linear regression

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}\theta_j^2\right]$$

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

Gradient descent

Repeat {

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

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

$(j = 1, 2, 3, \ldots, n)$

}

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

$1 - \alpha \frac{\lambda}{m} < 1$

0.99

$\theta_j \times 0.99$

Normal equation

$$X = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \quad m \times (n+1)$$

$$y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \quad \mathbb{R}^m$$

$$\min_\theta J(\theta)$$

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

$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

$(n+1) \times (n+1)$

e.g. $n = 2$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Non-invertibility (optional/advanced).

Suppose $m \leq n$,
(#examples) (#features)

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

non-invertible / singular

pinv

inv

If $\lambda > 0$,

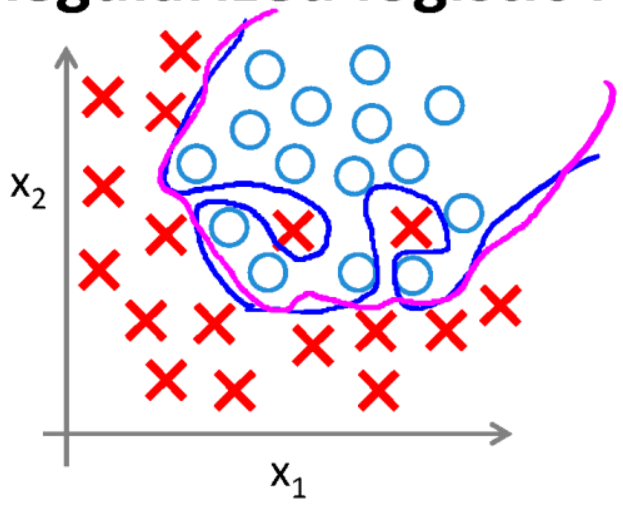
$$\theta = \left(X^T X + \lambda \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \\ & & & & 1 \end{bmatrix} \right)^{-1} X^T y$$

invertible.

Regularization

Regularized logistic regression

Regularized logistic regression.



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

$\theta_1, \theta_2, \dots, \theta_n$

Gradient descent

Repeat $\{$

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

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

$(j = 1, 2, 3, \ldots, n)$

$\theta_1 \ldots \theta_n$

$\}$

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

$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$

Advanced optimization

```
function [jVal, gradient] = costFunction(theta)
    jVal = [code to compute J(θ)];
    gradient(1) = [code to compute ∂/∂θ0 J(θ)];
    gradient(2) = [code to compute ∂/∂θ1 J(θ)];
    gradient(3) = [code to compute ∂/∂θ2 J(θ)];
    ⋮
    gradient(n+1) = [code to compute ∂/∂θn J(θ)];
```

$$J(\theta) = \left[-\frac{1}{m} \sum_{i=1}^{m} y^{(i)} \log\left(h_\theta(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log 1 - h_\theta(x^{(i)}) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

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

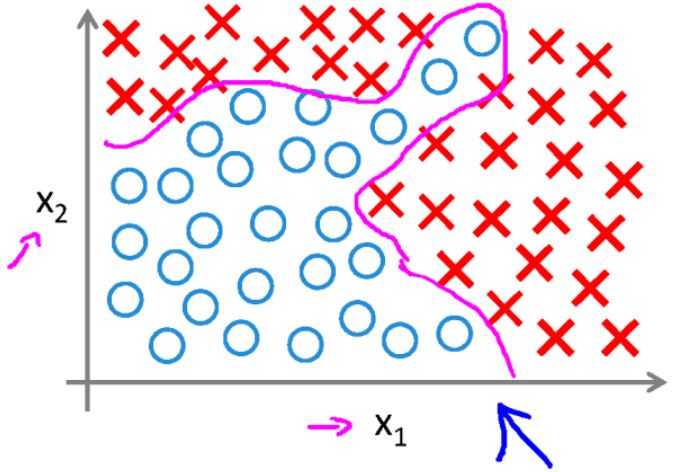
$$\left(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)} \right) - \frac{\lambda}{m}\theta_1$$

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

Neural Networks: Representation

Non-linear hypotheses

Non-linear Classification



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1 x_2 + \theta_4 x_1^2 x_2 + \theta_5 x_1^3 x_2 + \theta_6 x_1 x_2^2 + \dots)$$

x_1 = size
x_2 = # bedrooms
x_3 = # floors
x_4 = age
$\dots$
x_{100}

$n = 100$

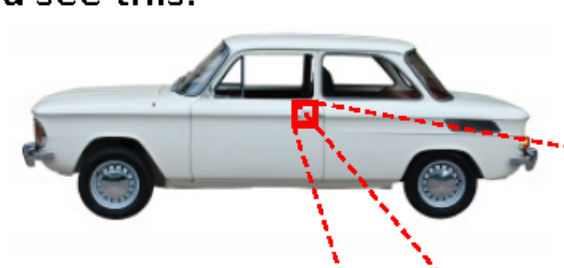
$x_1^2, x_1x_2, x_1x_3, x_1x_4 \dots x_1x_{100}$
$x_2^2, x_2x_3 \dots$
≈ 5000 feature $O(n^2)$

$x_1^2, x_2^2, x_3^2, \dots, x_{100}^2$ $\approx \frac{n^2}{2}$

$x_1x_2x_3, x_1^2x_2, x_{10}x_{11}x_{17}, \dots$
$O(n^3)$ 170,000

What is this?

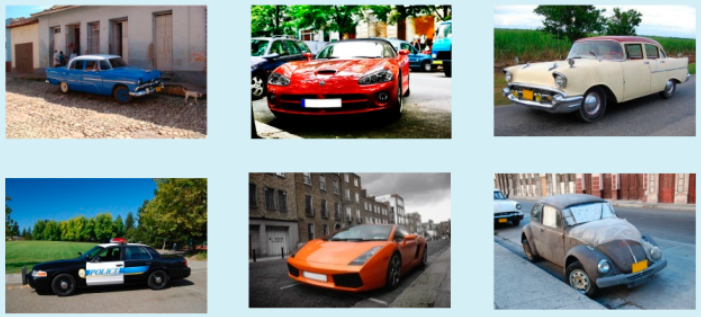
You see this:



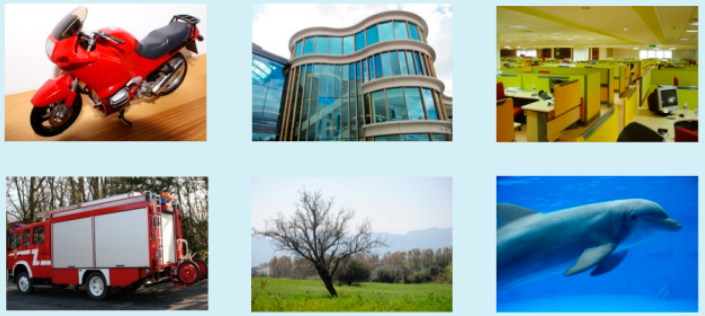
But the camera sees this:

194	210	201	212	199	213	215	195	178	158	182	209
180	189	190	221	209	205	191	167	147	115	129	163
114	126	140	188	176	165	152	140	170	106	78	88
87	103	115	154	143	142	149	153	173	101	57	57
102	112	106	131	122	138	152	147	128	84	58	66
94	95	79	104	105	124	129	113	107	87	69	67
68	71	69	98	89	92	98	95	89	88	76	67
41	56	68	99	63	45	60	82	58	76	75	65
20	43	69	75	56	41	51	73	55	70	63	44
50	50	57	69	75	75	73	74	53	68	59	37
72	59	53	66	84	92	84	74	57	72	63	42
67	61	58	65	75	78	76	73	59	75	69	50

Computer Vision: Car detection



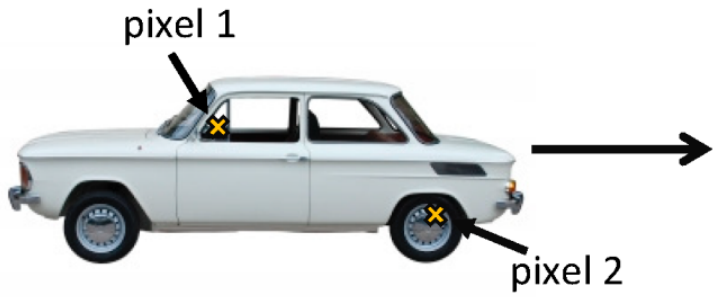
Cars



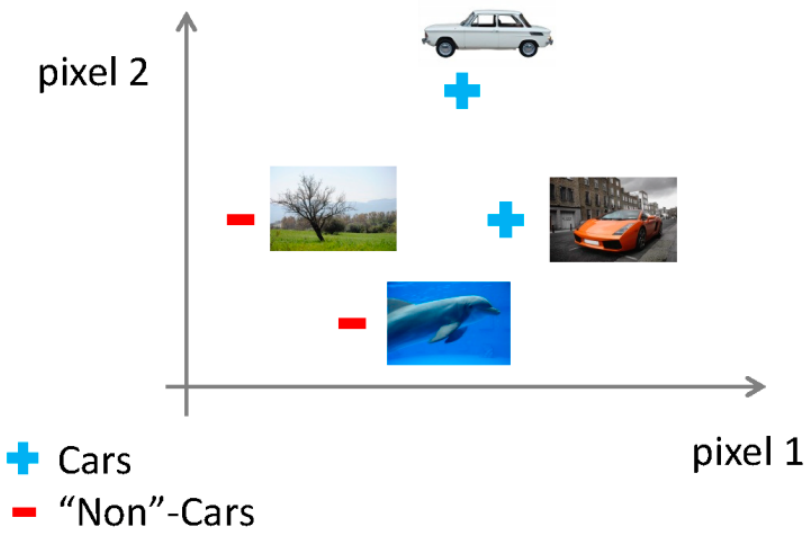
Not a car

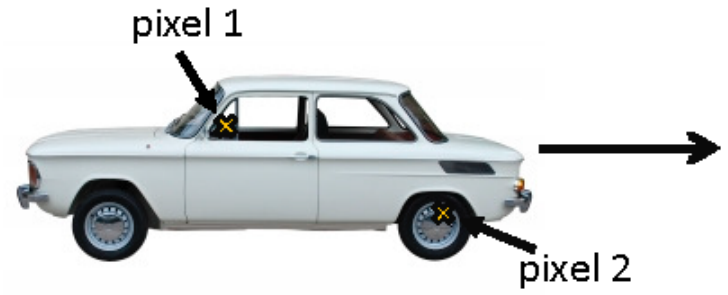
Testing:

What is this?

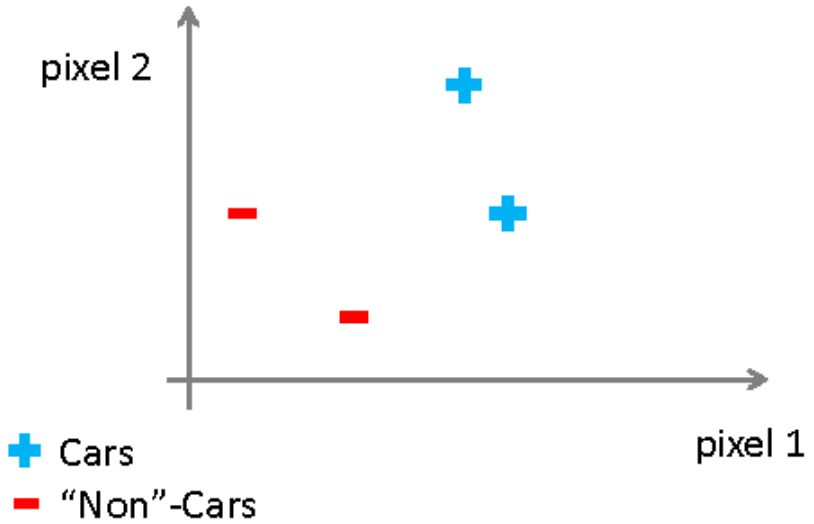


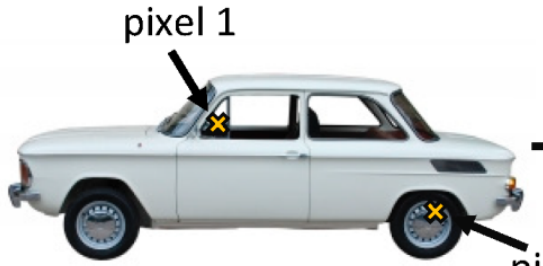
Learning Algorithm



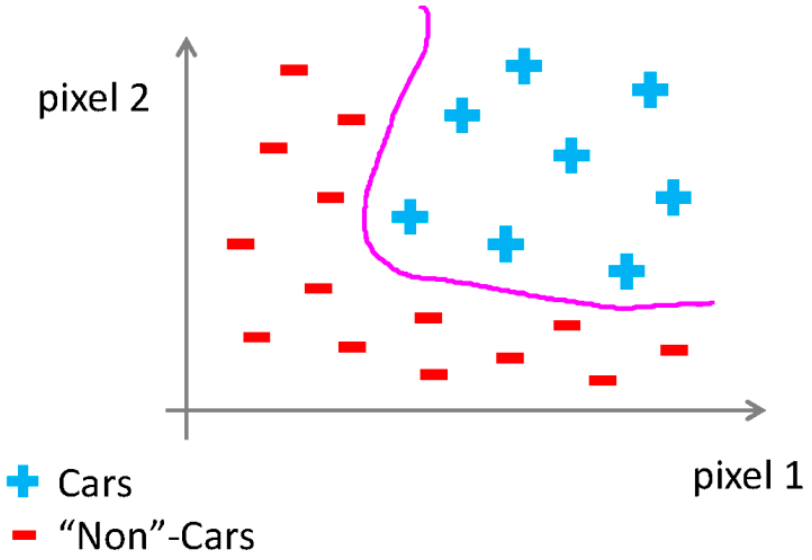


Learning Algorithm





Learning Algorithm



50 x 50 pixel images→ 2500 pixels

$n = 2500$ (7500 if RGB)

$$x = \begin{bmatrix} \text{pixel 1 intensity} \\ \text{pixel 2 intensity} \\ \vdots \\ \text{pixel 2500 intensity} \end{bmatrix}$$

0-255

Quadratic features ($x_i \times x_j$): ≈3 million features

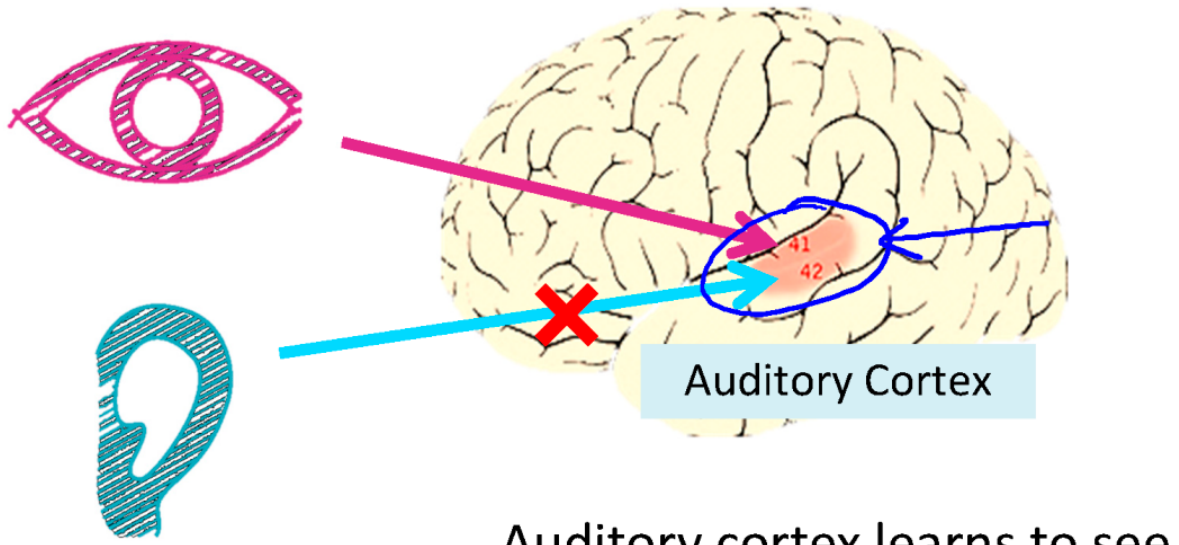
Neural Networks: Representation

Neurons and the brain

Neural Networks

- Origins: Algorithms that try to mimic the brain.
- Was very widely used in 80s and early 90s; popularity diminished in late 90s.
- Recent resurgence: State-of-the-art technique for many applications

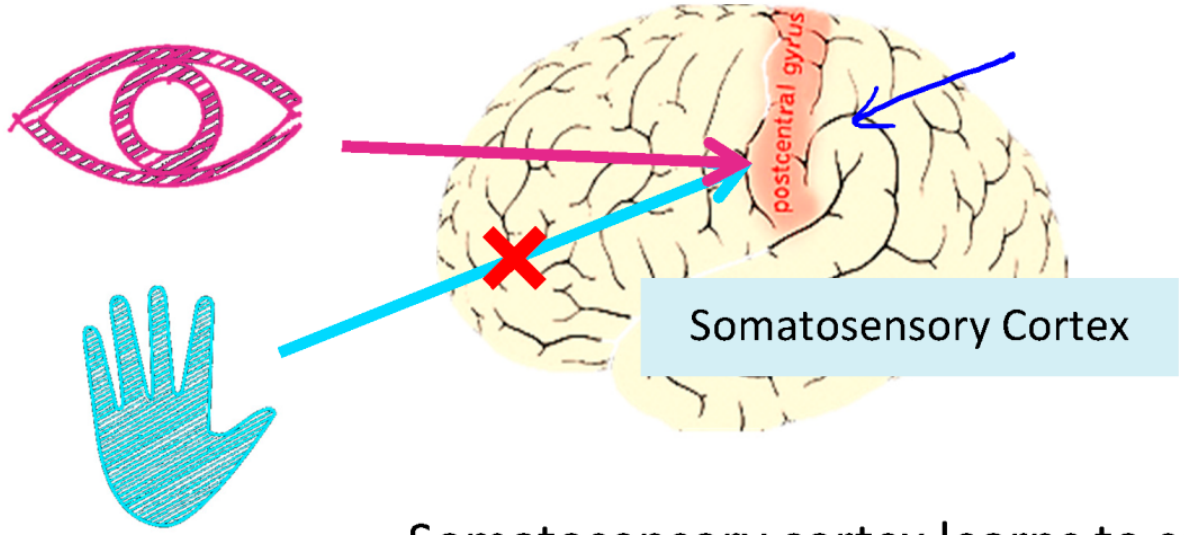
The “one learning algorithm” hypothesis



Auditory cortex learns to see

[Roe et al., 1992]

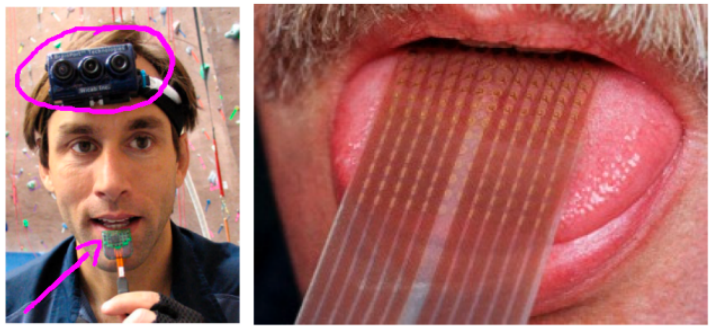
The “one learning algorithm” hypothesis



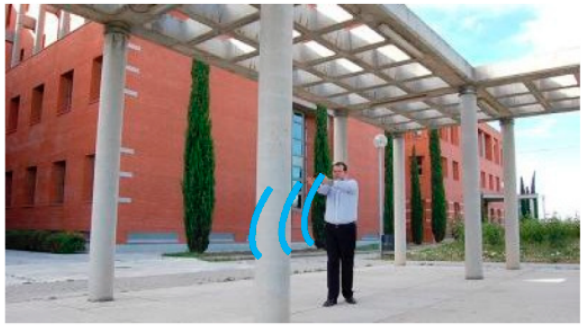
Somatosensory cortex learns to see

[Metin & Frost, 1989]

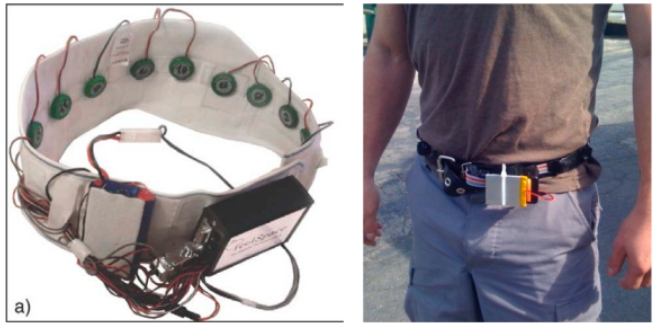
Sensor representations in the brain



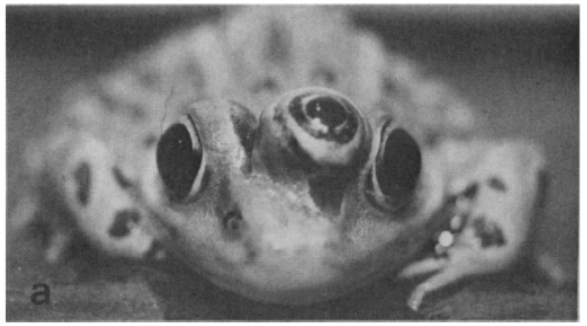
Seeing with your tongue



Human echolocation (sonar)



Haptic belt: Direction sense



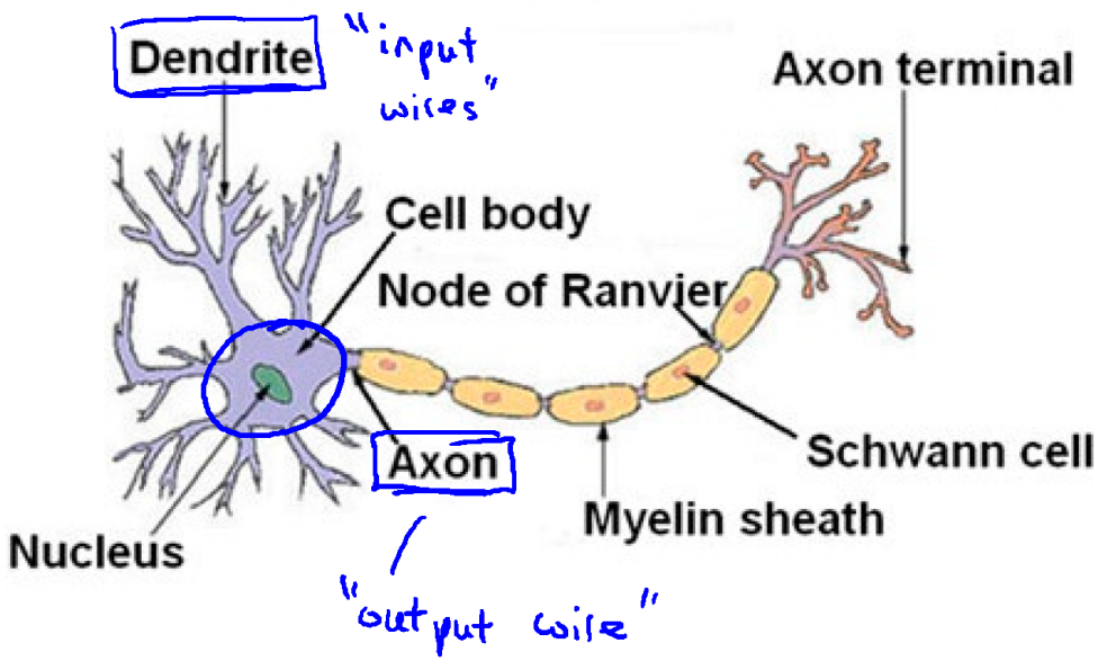
Implanting a 3rd eye

[BrainPort; Welsh & Blasch, 1997; Nagel et al., 2005; Constantine-Paton & Law, 2009]

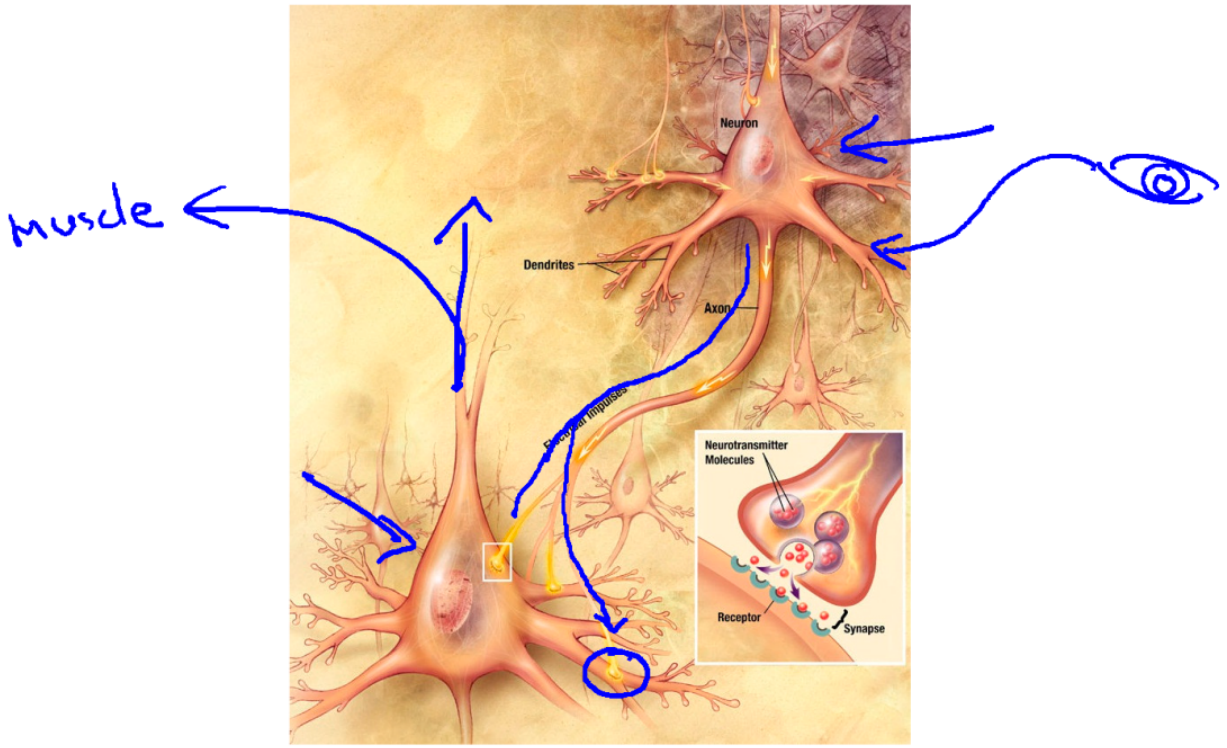
Neural Networks: Representation

Model representation I

Neuron in the brain

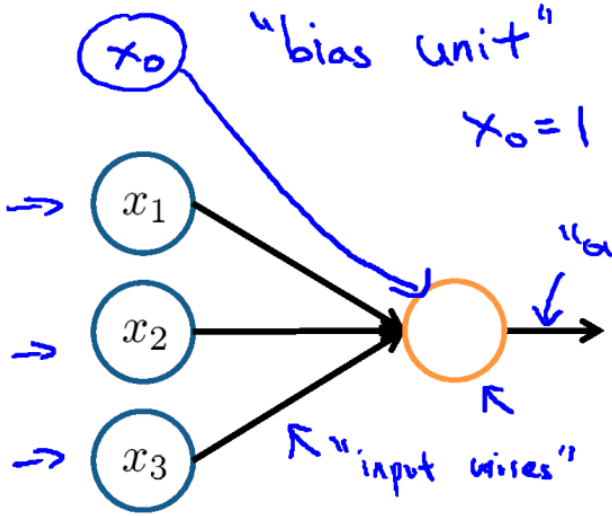


Neurons in the brain



[Credit: US National Institutes of Health, National Institute on Aging]

Neuron model: Logistic unit



$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

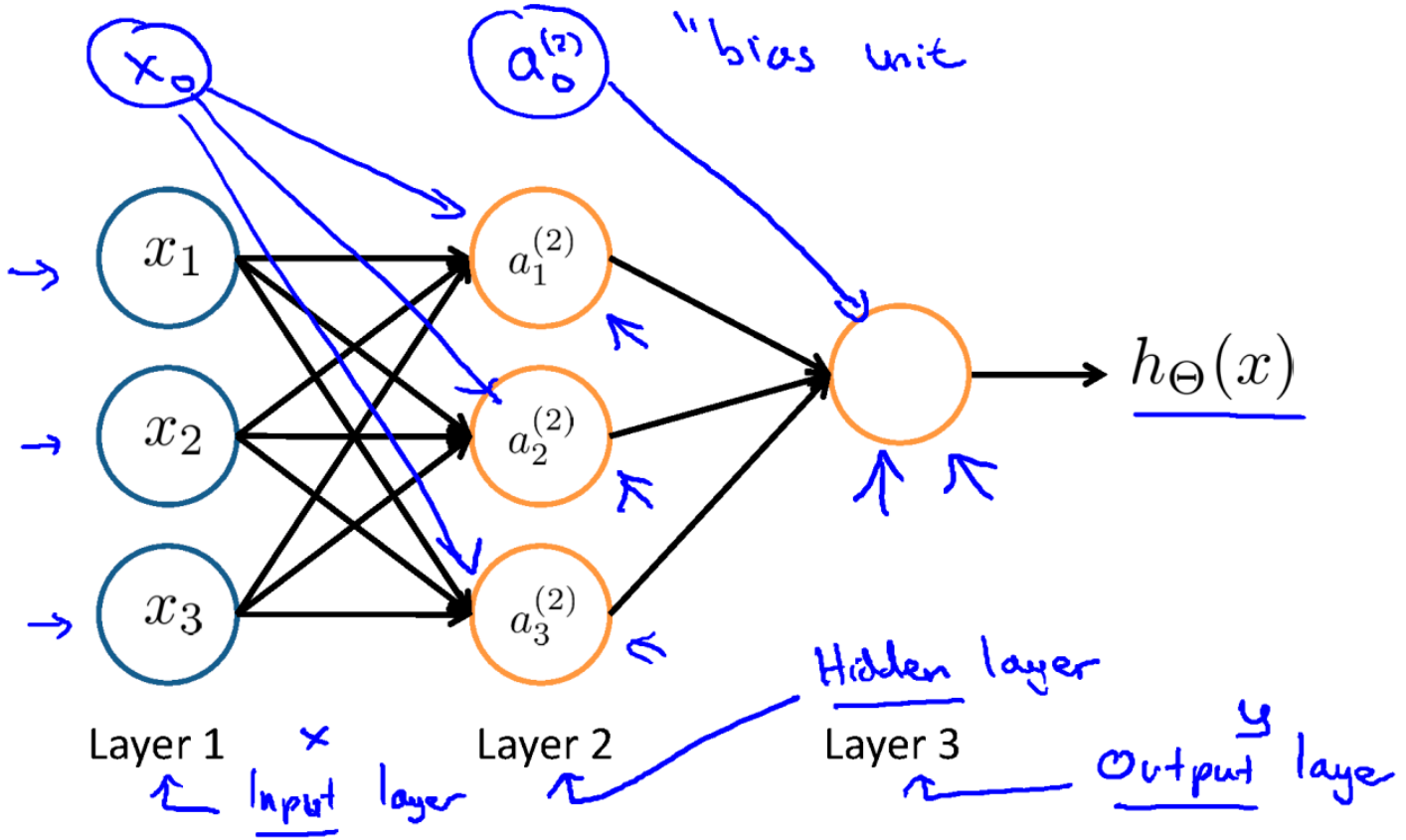
"weights" (parameters)

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

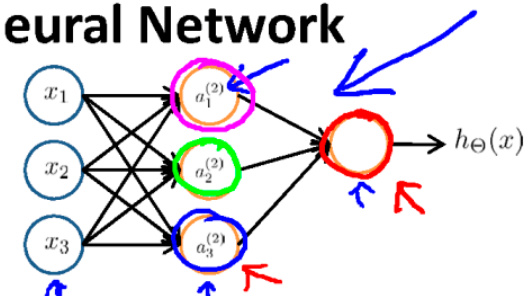
Sigmoid (logistic) activation function.

$$g(z) = \frac{1}{1 + e^{-z}}$$

Neural Network



Neural Network



→ $a_i^{(j)}$ = "activation" of unit i in layer j

→ $\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$

$\Theta^{(1)} \in \mathbb{R}^{3\times 4}$

$h_\Theta(x)$

→ $a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$

→ $a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$

→ $a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$

$\Theta^{(2)}$

→ $h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$

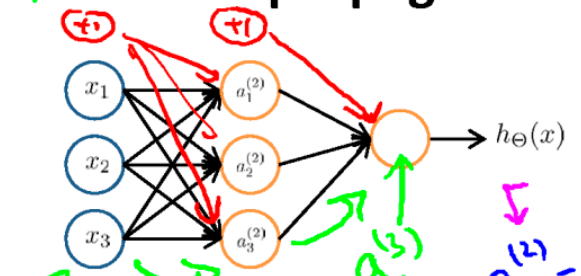
→ If network has s_j units in layer j, s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

$s_{j+1} \times (s_j + 1)$

Neural Networks: Representation

Model representation II

Forward propagation: Vectorized implementation



$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$
$$h_\Theta(x) = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

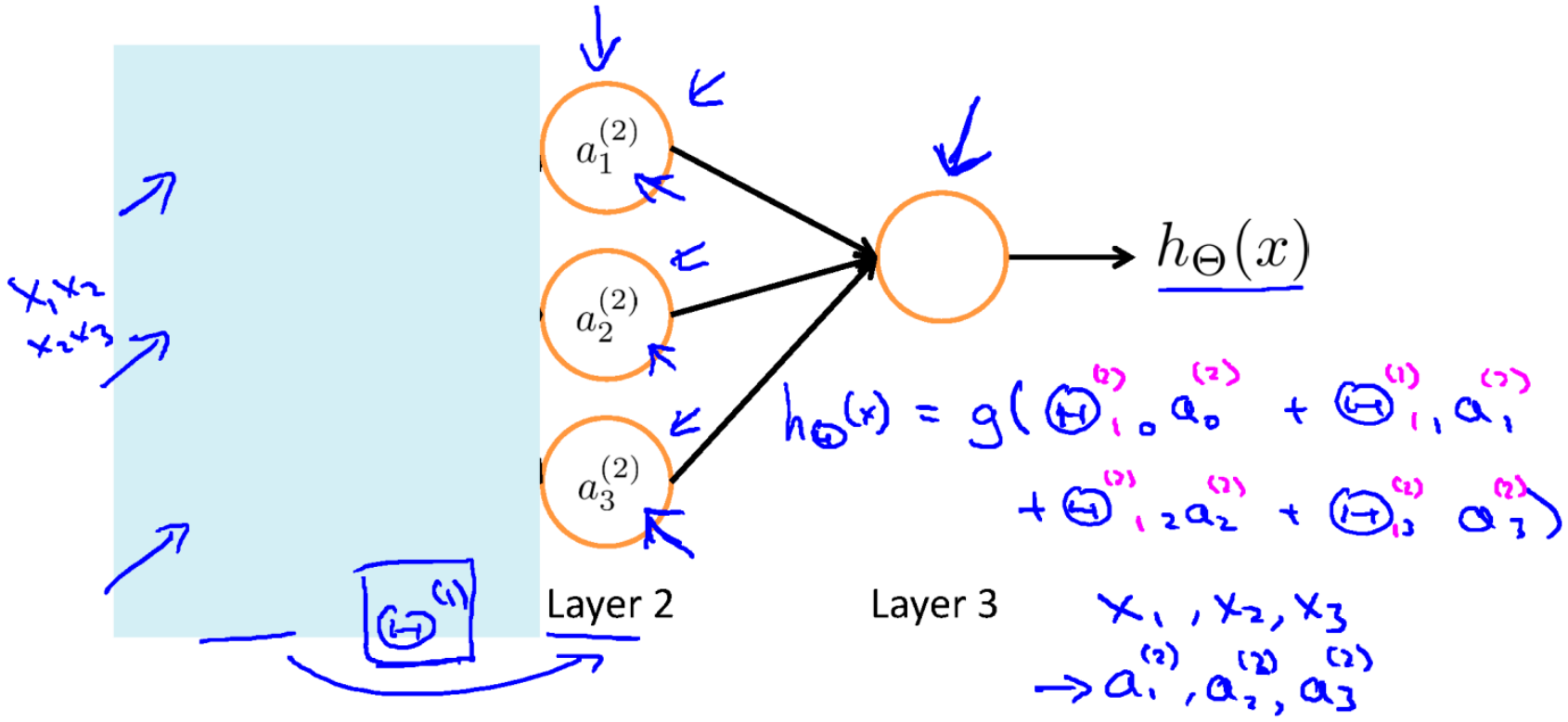
$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad z^{(2)} = \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix}$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$
$$a^{(2)} = g(z^{(2)})$$

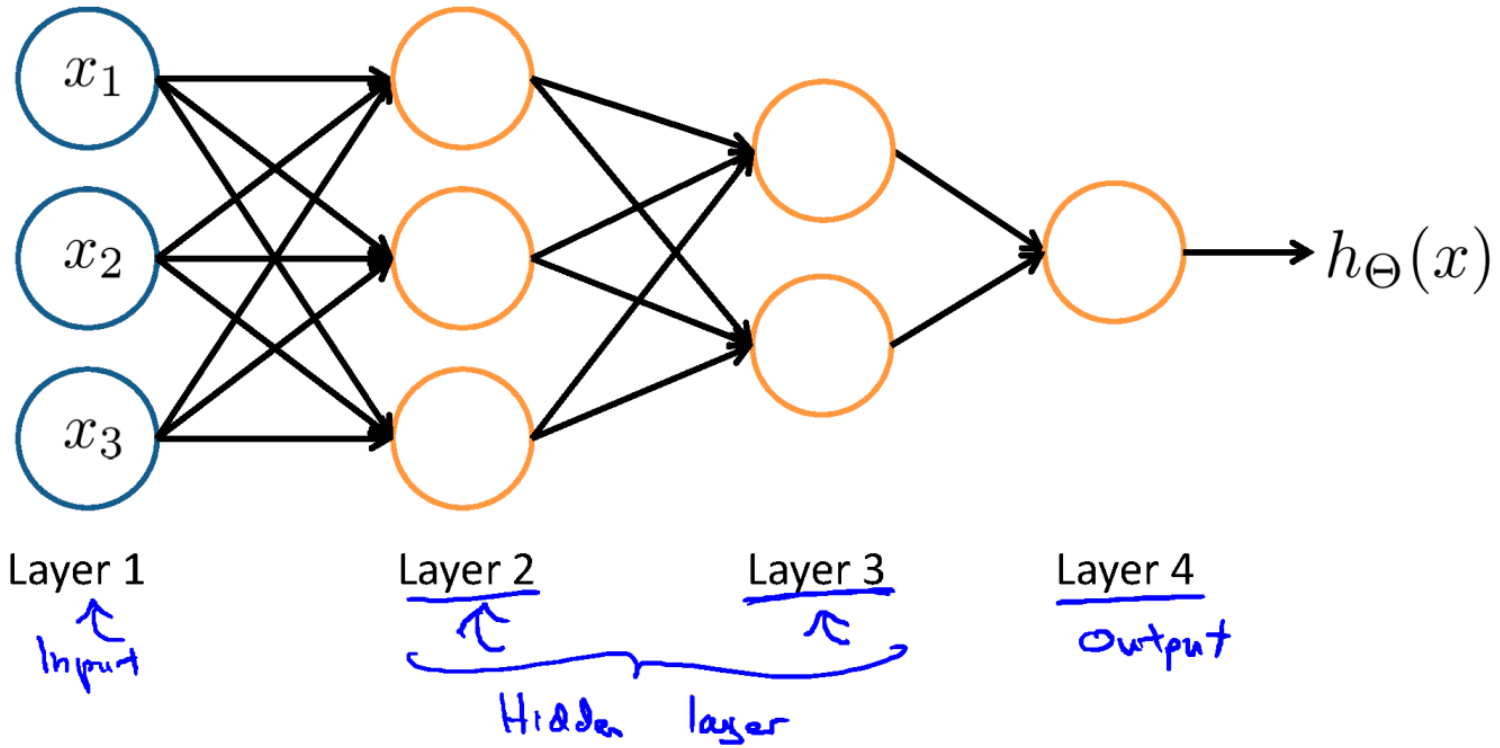
Add $a_0^{(2)} = 1.$ → $a^{(2)} \in \mathbb{R}^4$

$$z^{(3)} = \Theta^{(2)} a^{(2)}$$
$$h_\Theta(x) = a^{(3)} = g(z^{(3)})$$

Neural Network learning its own features



Other network architectures

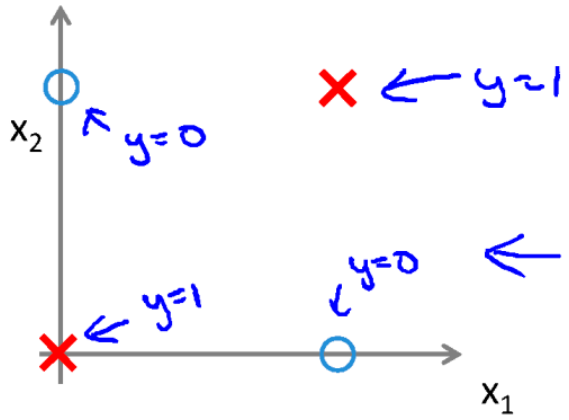


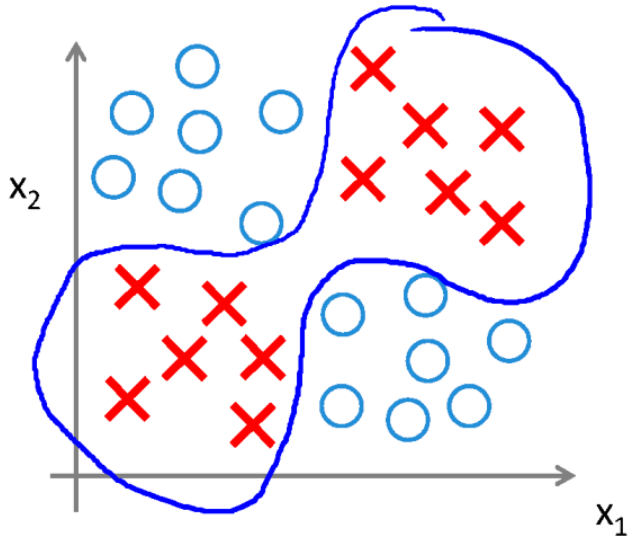
Neural Networks: Representation

Examples and intuitions I

Non-linear classification example: XOR/XNOR

x_1, x_2 are binary (0 or 1).





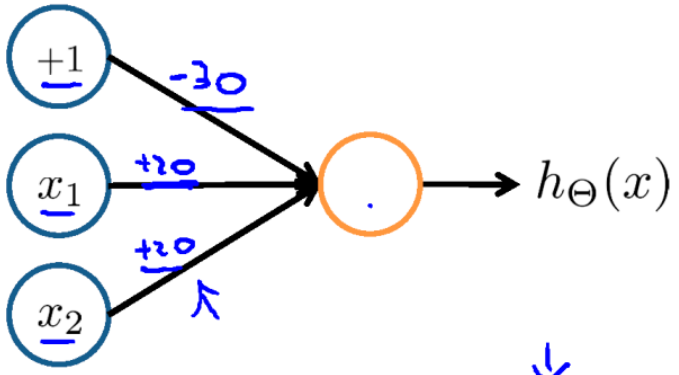
$y = x_1 \text{ XOR } x_2$

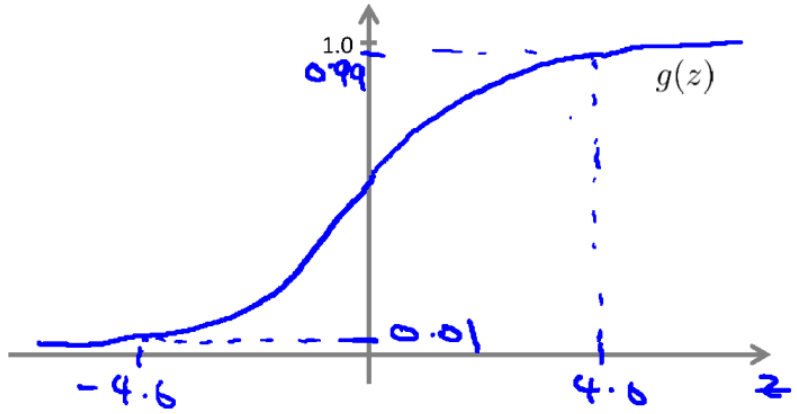
$x_1 \text{ XNOR } x_2$

$\text{NOT } (x_1 \text{ XOR } x_2)$

Simple example: AND

- $x_1, x_2 \in \{0, 1\}$
- $y = x_1$ AND x_2





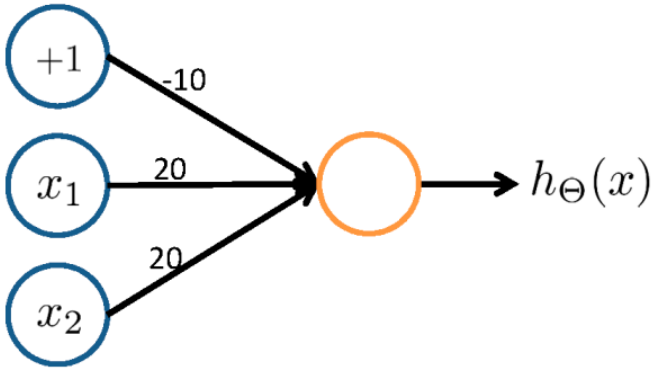
$h_\Theta(x) = g(-30 + 20x_1 + 20x_2)$

$\Theta^{(1)}_{10}$ $\Theta^{(1)}_{11}$ $\Theta^{(1)}_{12}$

x_1	x_2	$h_\Theta(x)$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

$h_\Theta(x) \approx x_1$ AND x_2

Example: OR function



$g(-10 + 20x_1 + 20x_2)$

x_1	x_2	$h_\Theta(x)$
0	0	$g(-10) \approx 0$
0	1	$g(10) \approx 1$
1	0	≈ 1
1	1	≈ 1

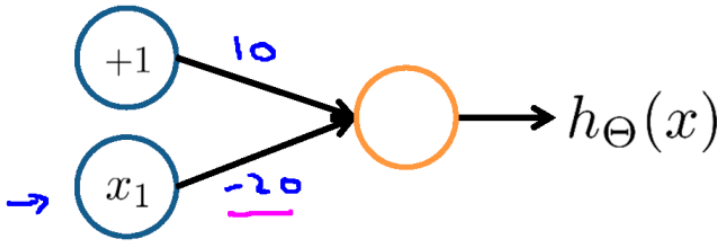
Neural Networks: Representation

Examples and intuitions II

→ x_1 AND x_2 → x_1 OR x_2 {0,1}.

Negation:

NOT x_1



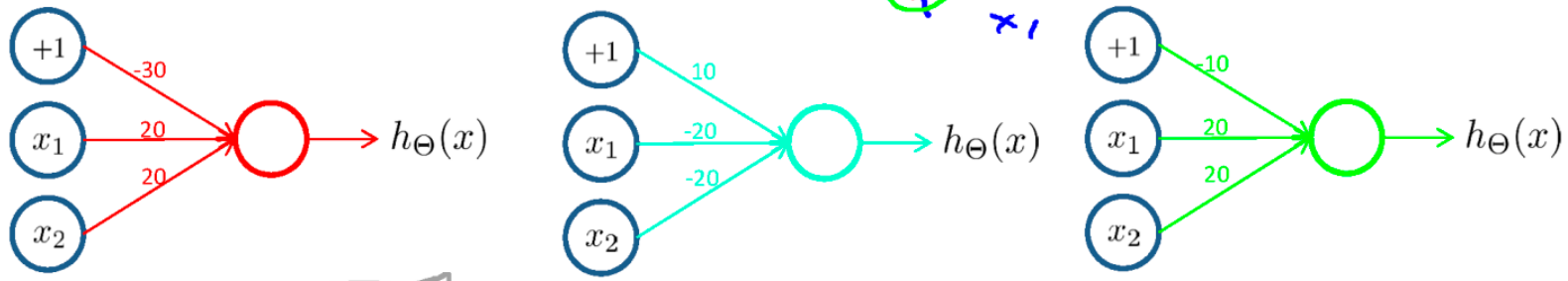
x_1	$h_\Theta(x)$
0	$g(10) \approx 1$
1	$g(-10) \approx 0$

$h_\Theta(x) = g(10 - 20x_1)$

→ (NOT x_1) AND (NOT x_2)

(=1 if and only if → $x_1 = x_2 = 0$

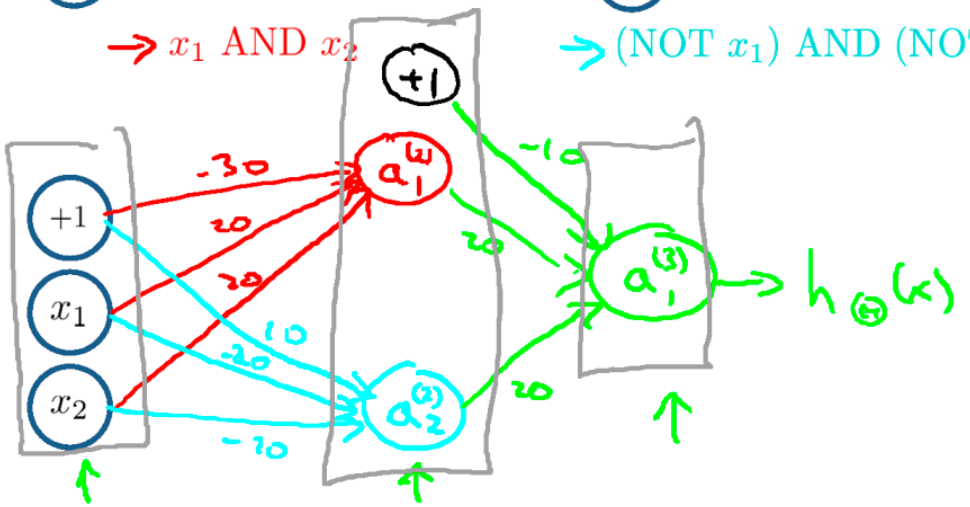
Putting it together: x_1 XNOR x_2



→ x_1 AND x_2

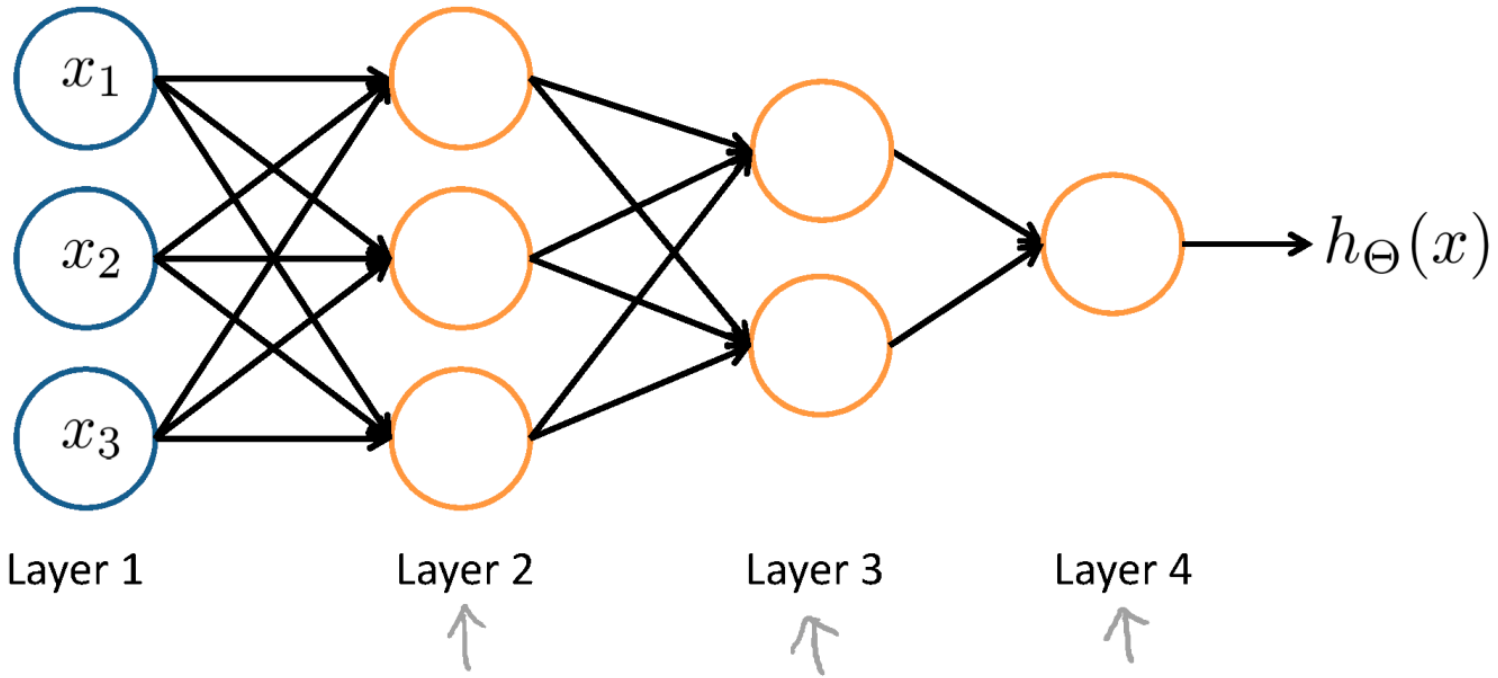
→ (NOT x_1) AND (NOT x_2)

→ x_1 OR x_2

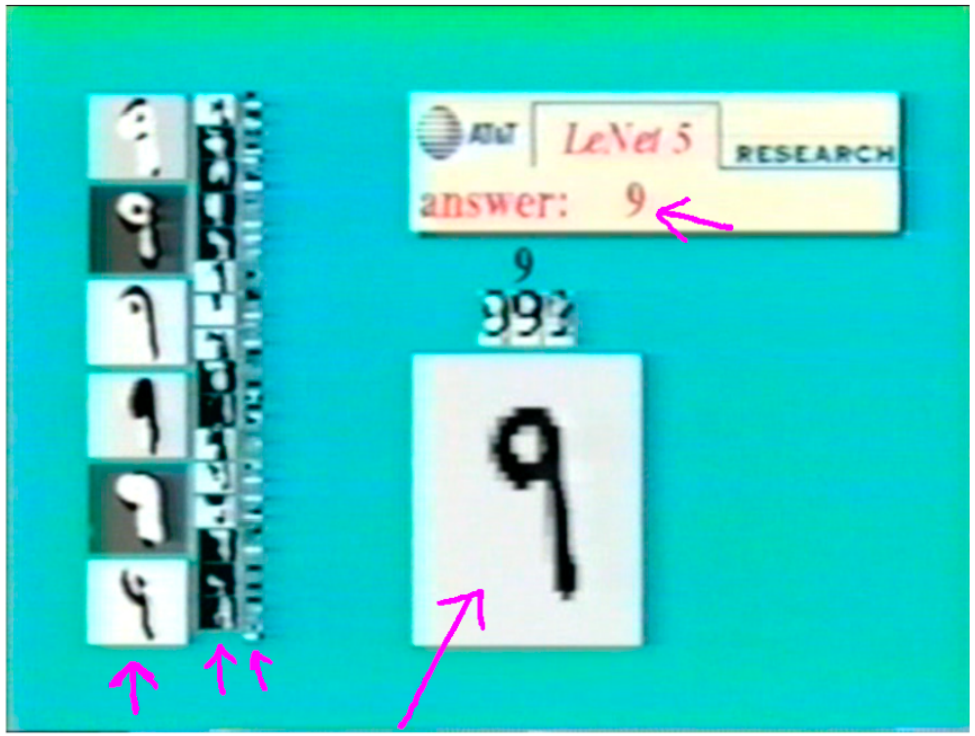


x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
0	0	0	1	1
0	1	0	0	0
1	0	0	0	0
1	1	1	0	1

Neural Network intuition

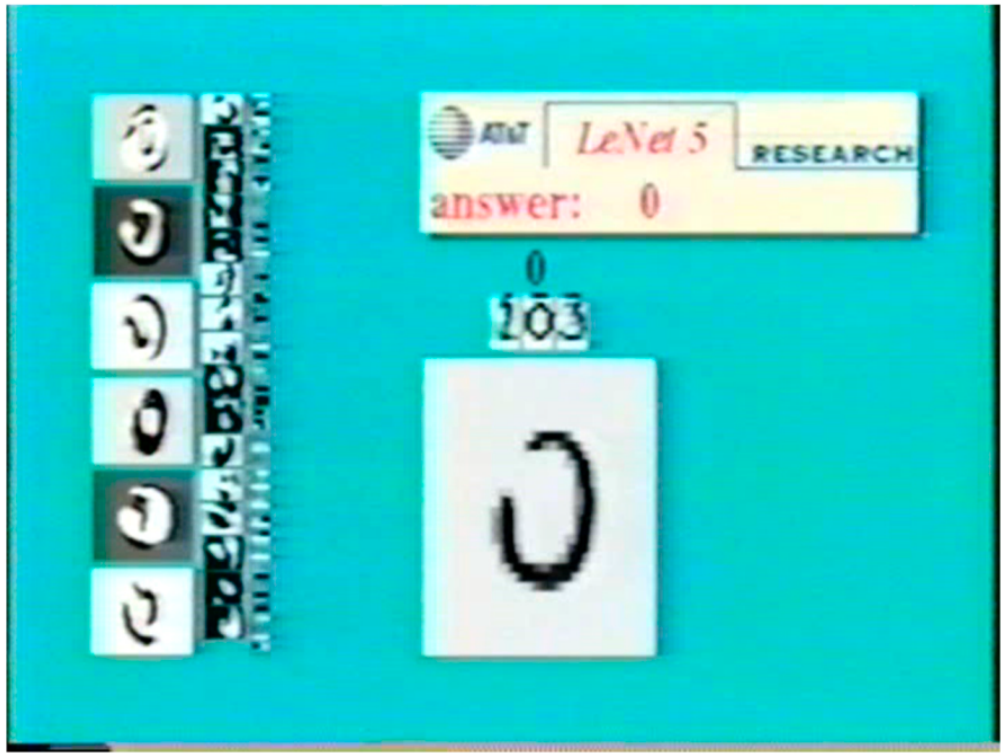


Handwritten digit classification



[Courtesy of Yann LeCun]

Handwritten digit classification



[Courtesy of Yann LeCun]

Neural Networks: Representation

Multi-class classification

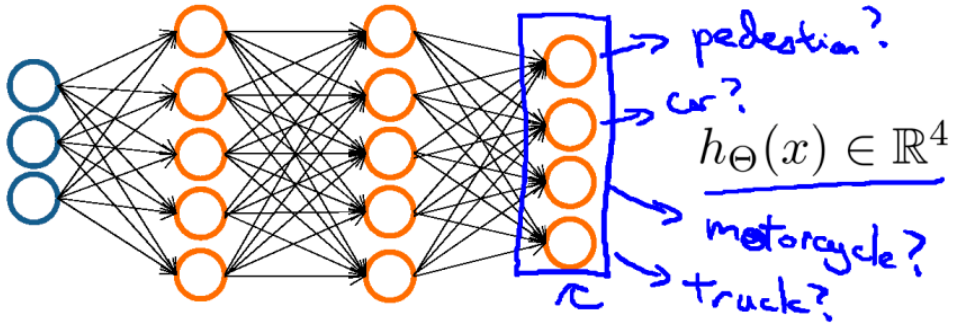
Multiple output units: One-vs-all.

Pedestrian

Car

Motorcycle

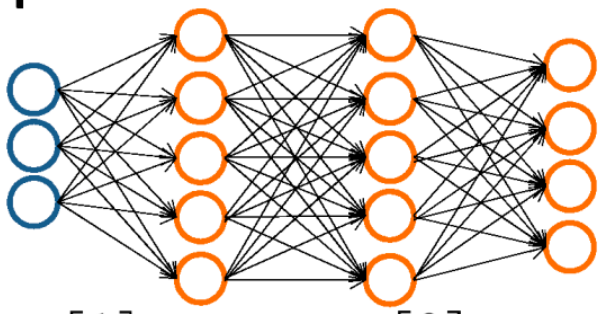
Truck



Want $h_\Theta(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, etc.

when pedestrian | when car | when motorcycle

Multiple output units: One-vs-all.



$h_\Theta(x) \in \mathbb{R}^4$

Want $h_\Theta(x) \approx \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, etc.

when pedestrian when car when motorcycle

Training set: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

$y^{(i)}$ one of $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

Previously $y \in \{1, 2, 3, 4\}$

$(x^{(i)}, y^{(i)})$

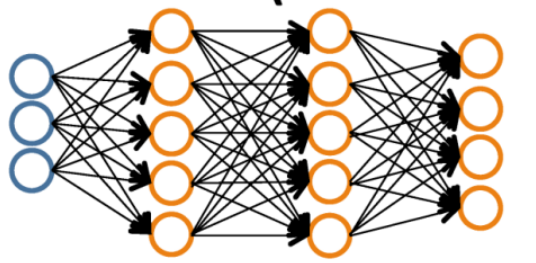
$h_\Theta(x^{(i)}) \approx y^{(i)}$

$\in \mathbb{R}^4$

Neural Networks: Learning

Cost function

Neural Network (Classification)



$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$

$L =$ total no. of layers in network

$s_l =$ no. of units (not counting bias unit) in layer l

Binary classification

$y = 0$ or 1

1 output unit

Multi-class classification (K classes)

$y \in \mathbb{R}^K$ E.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

K output units

Cost function

Logistic regression:

$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

Neural network:

$$h_\Theta(x) \in \mathbb{R}^K \quad (h_\Theta(x))_i = i^{th} \text{ output}$$

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log((h_\Theta(x^{(i)}))_k + (1 - y_k^{(i)}) \log(1 - (h_\Theta(x^{(i)}))_k)\right]$$

$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{ji}^{(l)})^2$$

Neural Networks: Learning

Backpropagationalgorithm

Gradient computation

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log h_\theta(x^{(i)})_k + (1 - y_k^{(i)}) \log(1 - h_\theta(x^{(i)})_k)\right]$$
$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_j^{(l)})^2$$

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

Need code to compute:

- $J(\Theta)$
- $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

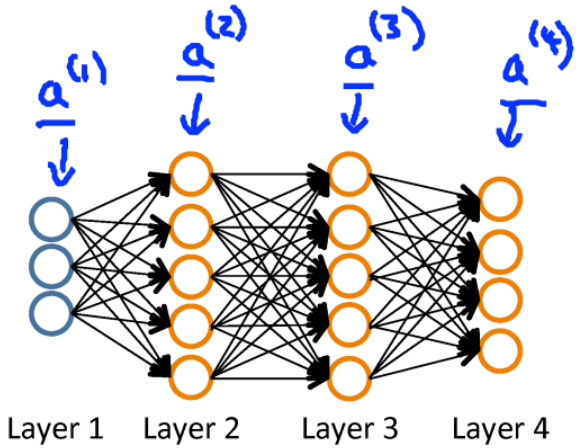
$\Theta_{ij}^{(l)} \in \mathbb{R}$

Gradient computation

Given one training example (x, y):

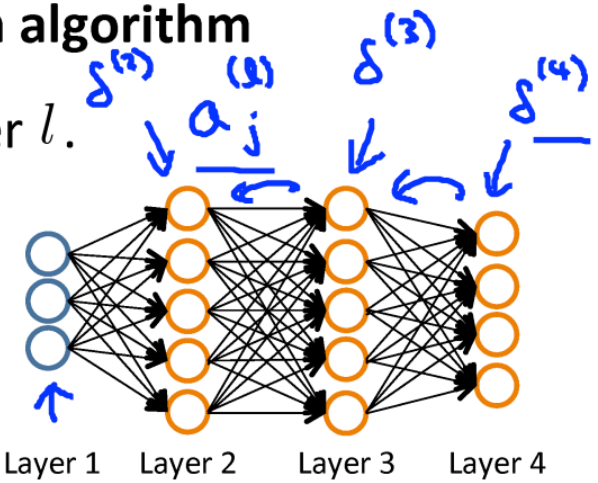
Forward propagation:

$$a^{(1)} = x$$
$$z^{(2)} = \Theta^{(1)} a^{(1)}$$
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$
$$z^{(3)} = \Theta^{(2)} a^{(2)}$$
$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$
$$z^{(4)} = \Theta^{(3)} a^{(3)}$$
$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



Gradient computation: Backpropagation algorithm

Intuition: $\delta_j^{(l)}$ = "error" of node j in layer l.



For each output unit (layer L = 4)

$$\delta_j^{(4)} = a_j^{(4)} - y_j$$

$$\delta^{(3)} = (\Theta^{(3)})^T \delta^{(4)} .* g'(z^{(3)})$$

$$\delta^{(2)} = (\Theta^{(2)})^T \delta^{(3)} .* g'(z^{(2)})$$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$

(ignore λ; if $\lambda = 0$)

Backpropagation algorithm

Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$

Set $\triangle_{ij}^{(l)} = 0$ (for all l, i, j).

(used to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$)

For $i = 1$ to m ← $(x^{(i)}, y^{(i)})$

Set $a^{(1)} = x^{(i)}$

Perform forward propagation to compute $a^{(l)}$ for $l = 2, 3, \ldots, L$

Using $y^{(i)}$, compute $\delta^{(L)} = a^{(L)} - y^{(i)}$

Compute $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$

$\triangle_{ij}^{(l)} := \triangle_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

$\triangle^{(l)} := \triangle^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

$$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} \quad \text{if } j \neq 0$$

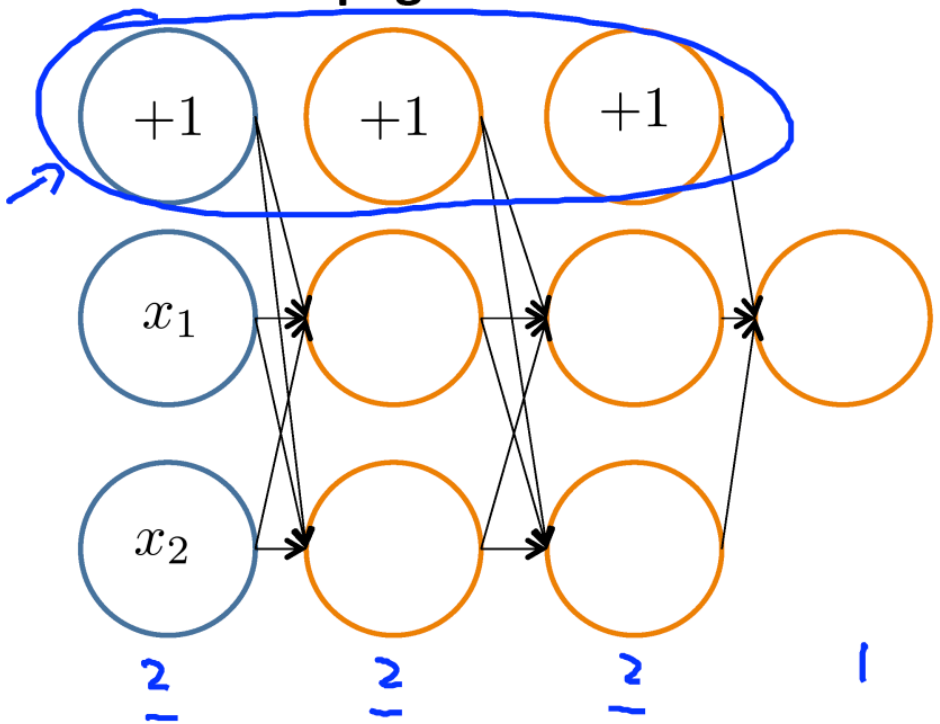
$$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} \quad \text{if } j = 0$$

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)}$$

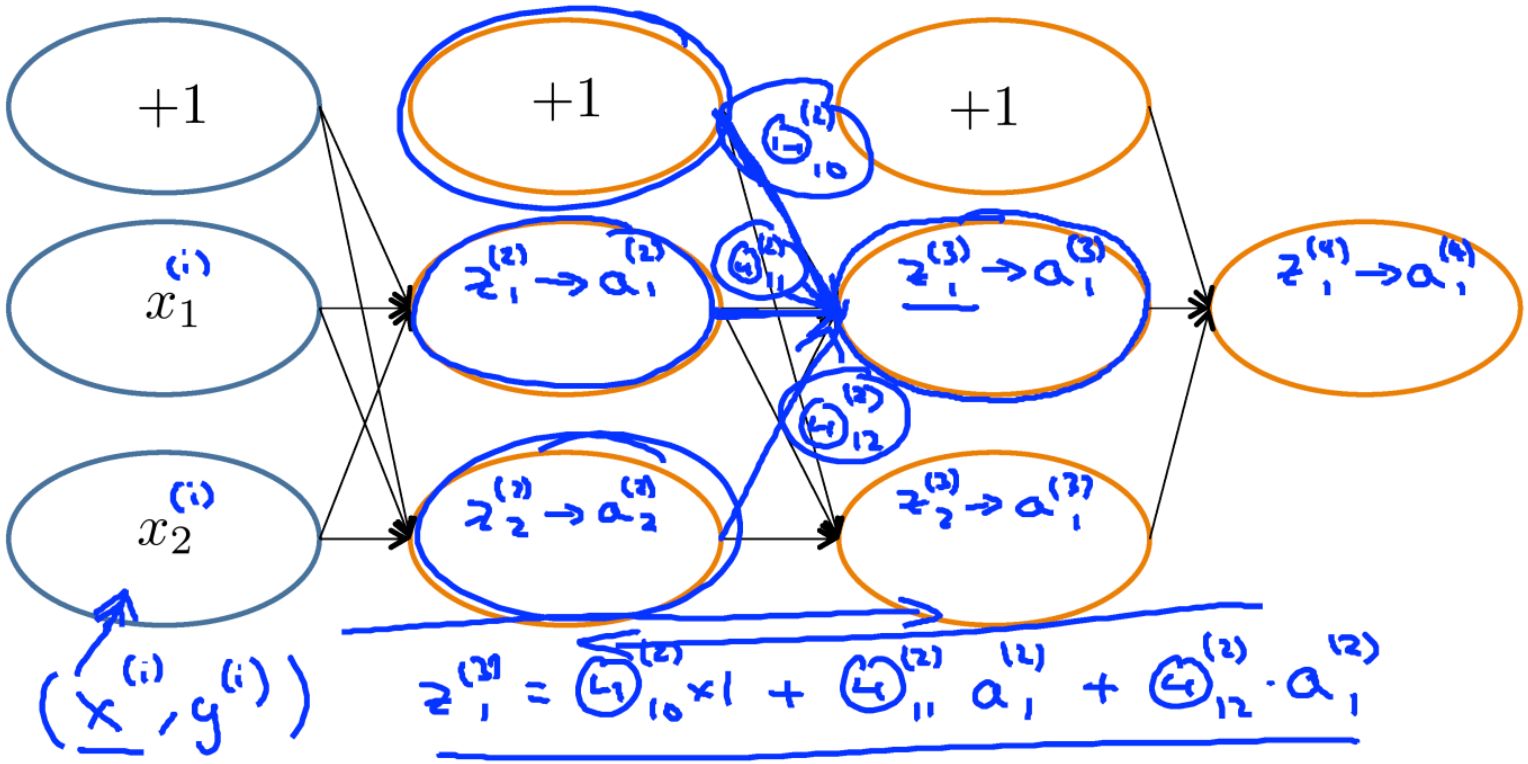
Neural Networks: Learning

Backpropagation intuition

Forward Propagation



Forward Propagation



What is backpropagation doing?

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \log(h_\Theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - (h_\Theta(x^{(i)})))\right] + \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{ji}^{(l)})^2$$

$(x^{(i)}, y^{(i)})$

Focusing on a single example $x^{(i)}$, $y^{(i)}$, the case of 1 output unit, and ignoring regularization ($\lambda = 0$),

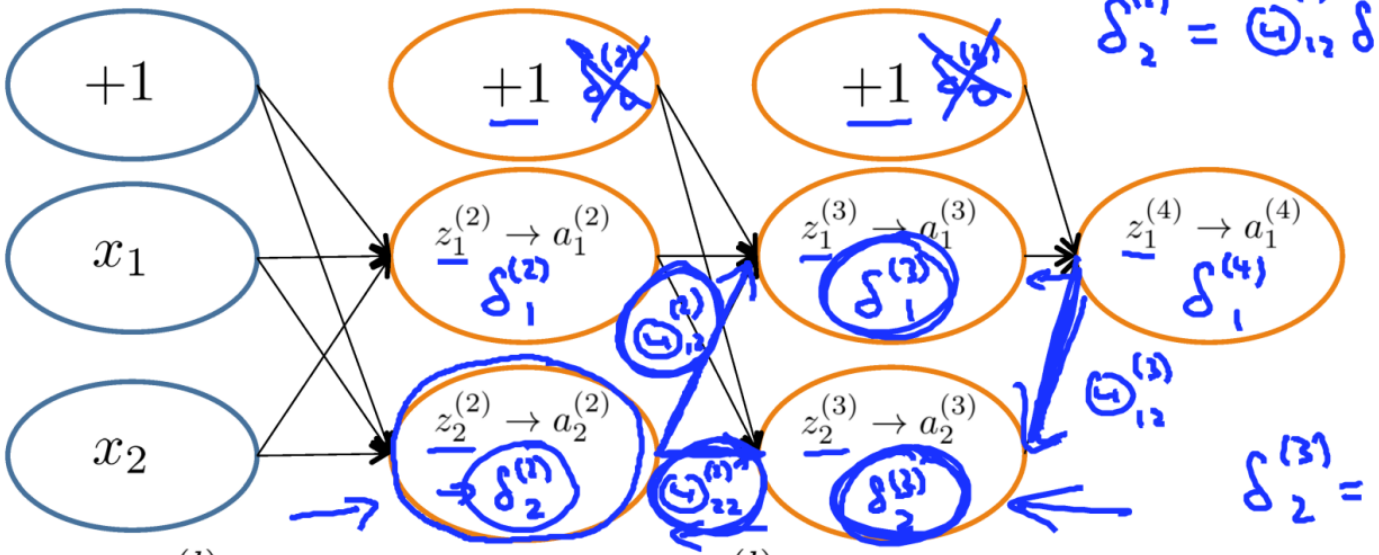
$$\text{cost(i)} = y^{(i)} \log h_\Theta(x^{(i)}) + (1 - y^{(i)}) \log h_\Theta(x^{(i)})$$

(Think of $\text{cost(i)} \approx (h_\Theta(x^{(i)}) - y^{(i)})^2$)

I.e. how well is the network doing on example i?

$y^{(i)}$

Forward Propagation



$\delta_j^{(l)}$ = "error" of cost for $a_j^{(l)}$ (unit j in layer l).

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost(i)}$ (for $j \geq 0$), where

$$\text{cost(i)} = y^{(i)} \log h_\Theta(x^{(i)}) + (1 - y^{(i)}) \log h_\Theta(x^{(i)})$$

Neural Networks: Learning

Implementation note: Unrolling parameters

Advanced optimization

```
function [jVal, gradient] = costFunction(theta)
    ...
optTheta = fminunc(@costFunction, initialTheta, options)
```

Neural Network (L=4):

- $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$ - matrices (`Theta1`, `Theta2`, `Theta3`)
- $D^{(1)}, D^{(2)}, D^{(3)}$ - matrices (`D1`, `D2`, `D3`)

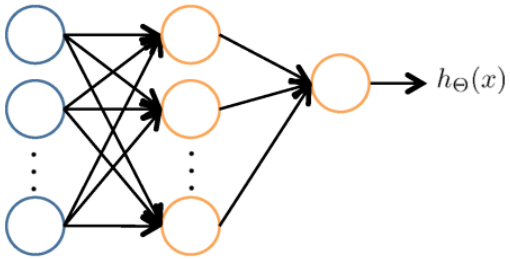
"Unroll" into vectors

Example

$s_1 = 10, s_2 = 10, s_3 = 1$

$\Theta^{(1)} \in \mathbb{R}^{10\times 11}, \Theta^{(2)} \in \mathbb{R}^{10\times 11}, \Theta^{(3)} \in \mathbb{R}^{1\times 11}$

$D^{(1)} \in \mathbb{R}^{10\times 11}, D^{(2)} \in \mathbb{R}^{10\times 11}, D^{(3)} \in \mathbb{R}^{1\times 11}$




```
thetaVec = [ Theta1(:); Theta2(:); Theta3(:)];
DVec = [D1(:); D2(:); D3(:)];

Theta1 = reshape(thetaVec(1:110),10,11);
Theta2 = reshape(thetaVec(111:220),10,11);
Theta3 = reshape(thetaVec(221:231),1,11);
```

Learning Algorithm

- Have initial parameters $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$.
- Unroll to get `initialTheta` to pass to
- `fminunc(@costFunction, initialTheta, options)`

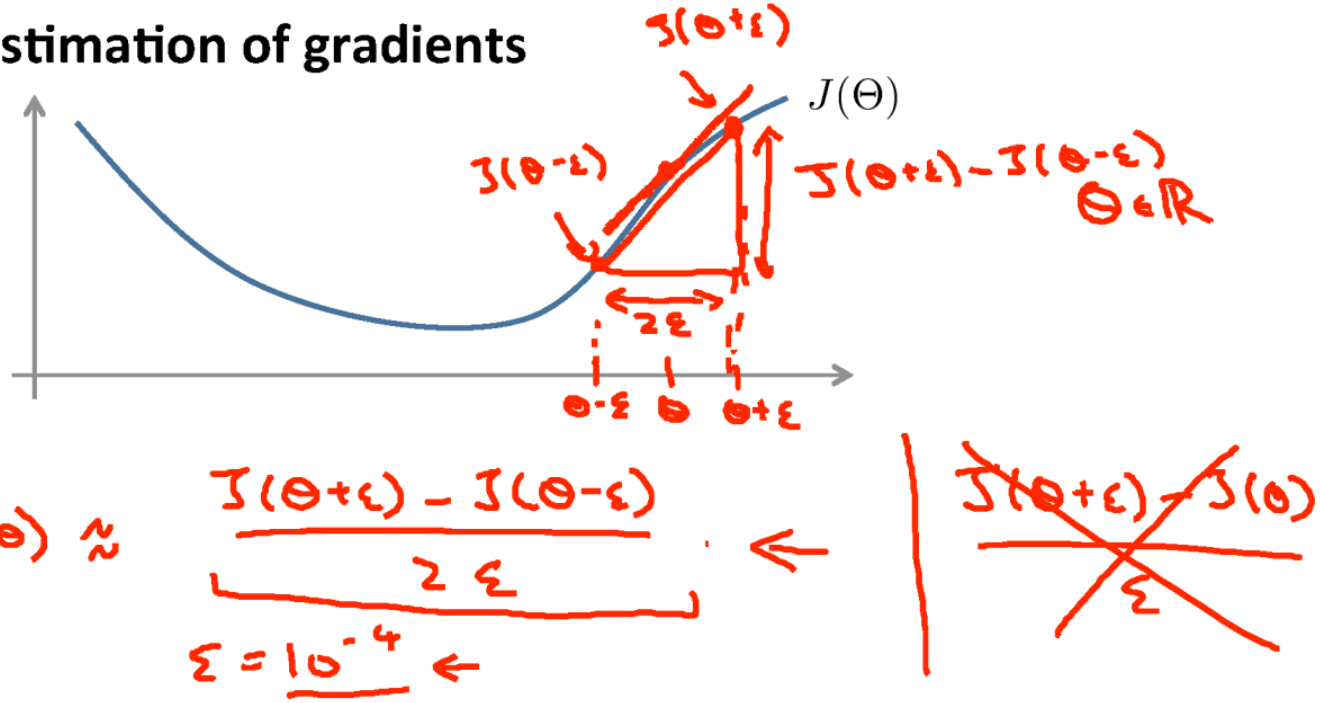
```
function [jval, gradientVec] = costFunction(thetaVec)
```

- From `thetaVec`, get $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$. reshape
- Use forward prop/back prop to compute $D^{(1)}, D^{(2)}, D^{(3)}$ $J(\Theta)$ and $D^{(1)}, D^{(2)}, D^{(3)}$
- Unroll to get `gradientVec`.

Neural Networks: Learning

Gradient checking

Numerical estimation of gradients



Implement: `gradApprox = (J(theta + EPSILON) - J(theta - EPSILON)) /(2*EPSILON)`

Parameter vector θ

- $\theta \in \mathbb{R}^n$ (E.g. θ is "unrolled" version of $\Theta^{(1)}, \Theta^{(2)}, \Theta^{(3)}$)
- $\theta = [\theta_1, \theta_2, \theta_3, \ldots, \theta_n]$
- $\frac{\partial}{\partial \theta_1} J(\theta) \approx \frac{J(\theta_1+\epsilon, \theta_2, \theta_3, \ldots, \theta_n) - J(\theta_1-\epsilon, \theta_2, \theta_3, \ldots, \theta_n)}{2\epsilon}$
- $\frac{\partial}{\partial \theta_2} J(\theta) \approx \frac{J(\theta_1, \theta_2+\epsilon, \theta_3, \ldots, \theta_n) - J(\theta_1, \theta_2-\epsilon, \theta_3, \ldots, \theta_n)}{2\epsilon}$
- $\vdots$
- $\frac{\partial}{\partial \theta_n} J(\theta) \approx \frac{J(\theta_1, \theta_2, \theta_3, \ldots, \theta_n+\epsilon) - J(\theta_1, \theta_2, \theta_3, \ldots, \theta_n-\epsilon)}{2\epsilon}$

```
for i = 1:n,
    thetaPlus = theta;
    thetaPlus(i) = thetaPlus(i) + EPSILON;
    thetaMinus = theta;
    thetaMinus(i) = thetaMinus(i) - EPSILON;
    gradApprox(i) = (J(thetaPlus) - J(thetaMinus))
                    /(2*EPSILON);
end;
```

$\theta = [\theta_1, \theta_2, \ldots, \theta_i + \varepsilon, \ldots, \theta_n] \rightarrow \theta_i - \varepsilon$

$\frac{\partial}{\partial \theta_i} J(\theta)$.

Check that gradApprox $\approx$ DVec

From back prop.

Implementation Note:

- Implement backprop to compute `DVec` (unrolled $D^{(1)}, D^{(2)}, D^{(3)}$).
- Implement numerical gradient check to compute `gradApprox`.
- Make sure they give similar values.
- Turn off gradient checking. Using backprop code for learning.

Important:

- Be sure to disable your gradient checking code before training your classifier. If you run numerical gradient computation on every iteration of gradient descent (or in the inner loop of `costFunction(...)`)your code will be very slow.

Neural Networks: Learning

Random initialization

Initial value of Θ

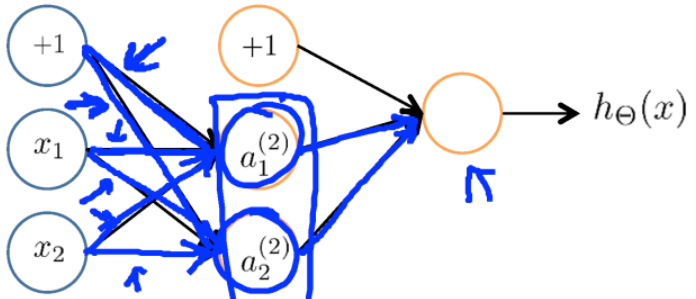
For gradient descent and advanced optimization method, need initial value for Θ.

```
optTheta = fminunc(@costFunction,
           initialTheta, options)
```

Consider gradient descent

Set `initialTheta = zeros(n,1)` ?

Zero initialization



$$\Rightarrow \Theta_{ij}^{(l)} = 0 \text{ for all } i, j, l.$$

$a_1^{(2)} = a_2^{(2)}$, Also $\delta_1^{(2)} = \delta_2^{(2)}$.

$\frac{\partial}{\partial \Theta_{01}^{(1)}} J(\Theta) = \frac{\partial}{\partial \Theta_{02}^{(1)}} J(\Theta)$ $\quad \Theta_{01}^{(1)} = \Theta_{02}^{(1)}$

After each update, parameters corresponding to inputs going into each of two hidden units are identical.

$a_1^{(2)} = a_2^{(2)}$

Random initialization: Symmetry breaking

Initialize each $\Theta_{ij}^{(l)}$ to a random value in $[-\epsilon, \epsilon]$
(i.e. $-\epsilon \leq \Theta_{ij}^{(l)} \leq \epsilon$)

E.g.

random 10×11 matrix (betw. 0 and 1)

```
Theta1 = rand(10,11)*(2*INIT_EPSILON)
         - INIT_EPSILON;
```

$[-\epsilon, \epsilon]$

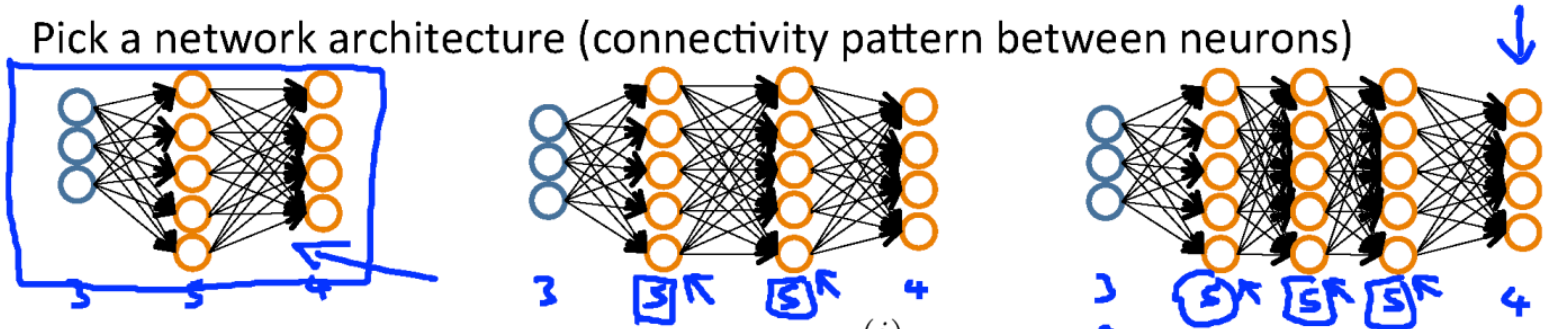
```
Theta2 = rand(1,11)*(2*INIT_EPSILON)
         - INIT_EPSILON;
```

Neural Networks: Learning

Putting it together

Training a neural network

Pick a network architecture (connectivity pattern between neurons)



- No. of input units: Dimension of features $x^{(i)}$
- No. output units: Number of classes

Reasonable default: 1 hidden layer, or if >1 hidden layer, have same no. of hidden units in every layer (usually the more the better)

$y \in \{1, 2, 3, \ldots, 10\}$

$y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ or $\begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ $\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$

Training a neural network

1. Randomly initialize weights
2. Implement forward propagation to get $h_\Theta(x^{(i)})$ for any $x^{(i)}$
3. Implement code to compute cost function $J(\Theta)$
4. Implement backprop to compute partial derivatives $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$

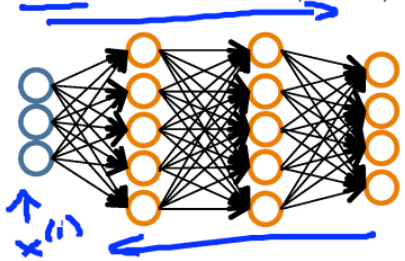
for i = 1:m {

- Perform forward propagation and backpropagation using example $(x^{(i)}, y^{(i)})$
  (Get activations $a^{(l)}$ and delta terms $\delta^{(l)}$ for $l = 2, \ldots, L$).

$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

}

Compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$.

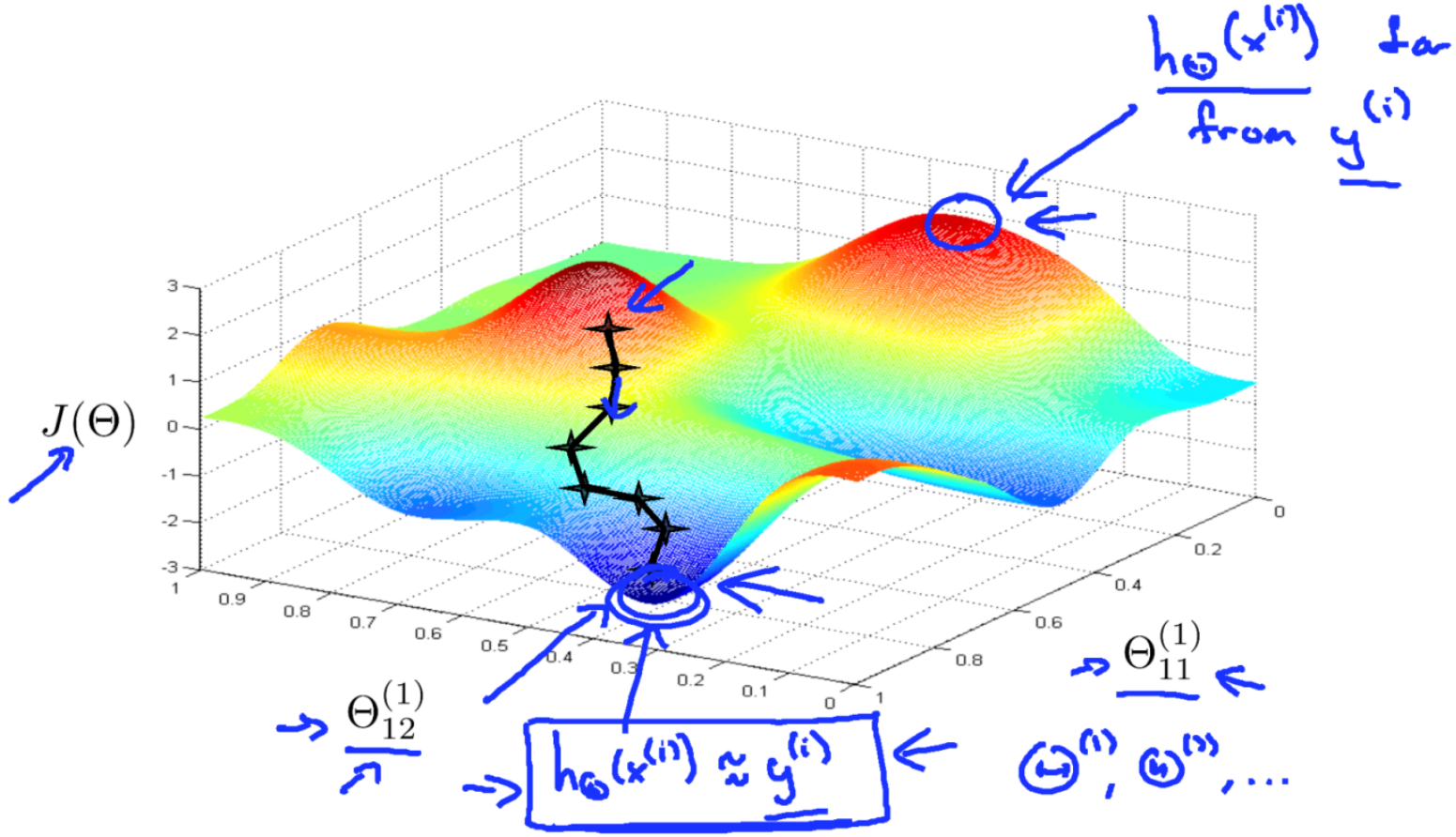


Training a neural network

5. Use gradient checking to compare $\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$ computed using backpropagation vs. using numerical estimate of gradient of $J(\Theta)$.
   - Then disable gradient checking code.
6. Use gradient descent or advanced optimization method with backpropagation to try to minimize $J(\Theta)$ as a function of parameters Θ

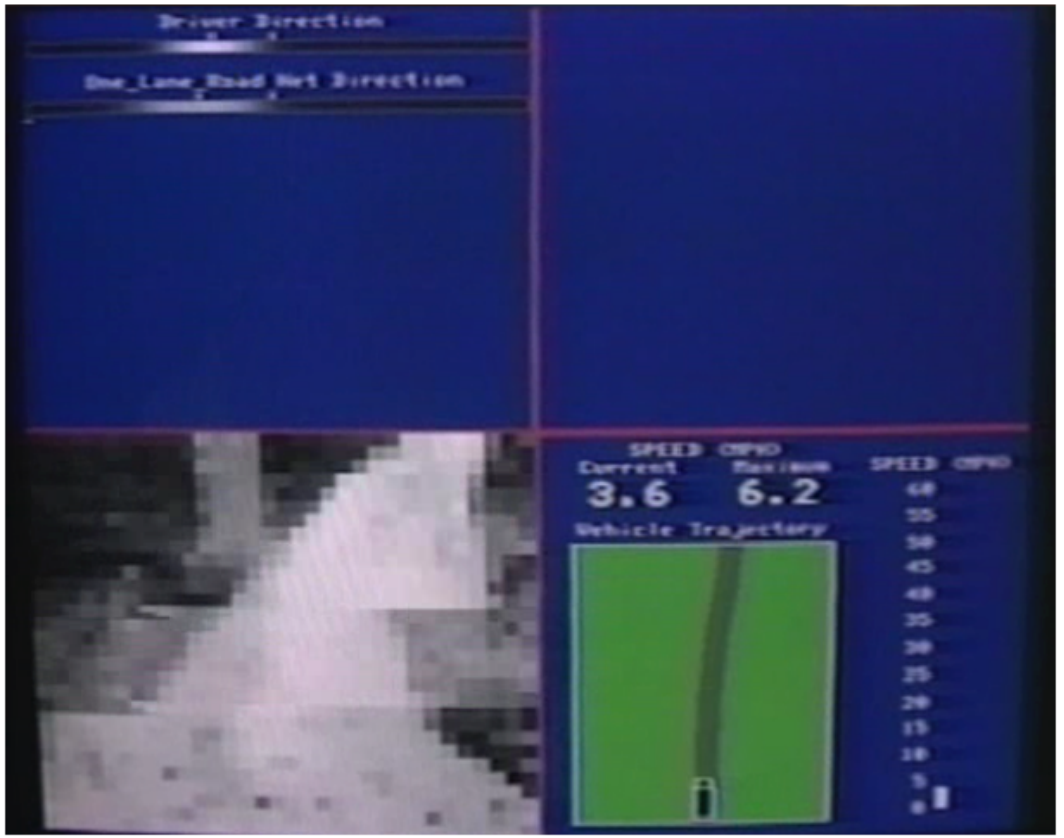
$\frac{\partial}{\partial \Theta_{jk}^{(l)}} J(\Theta)$

$J(\Theta)$ — non-convex.


$J(\Theta)$
$h_\Theta(x^{(i)})$ far from $y^{(i)}$
$\Theta_{12}^{(1)}$
$\Theta_{11}^{(1)}$
$h_\Theta(x^{(i)}) \approx y^{(i)}$
$\Theta^{(1)}, \Theta^{(2)}, \ldots$

Neural Networks: Learning

Backpropagation example: Autonomous driving (optional)



[Courtesy of Dean Pomerleau]