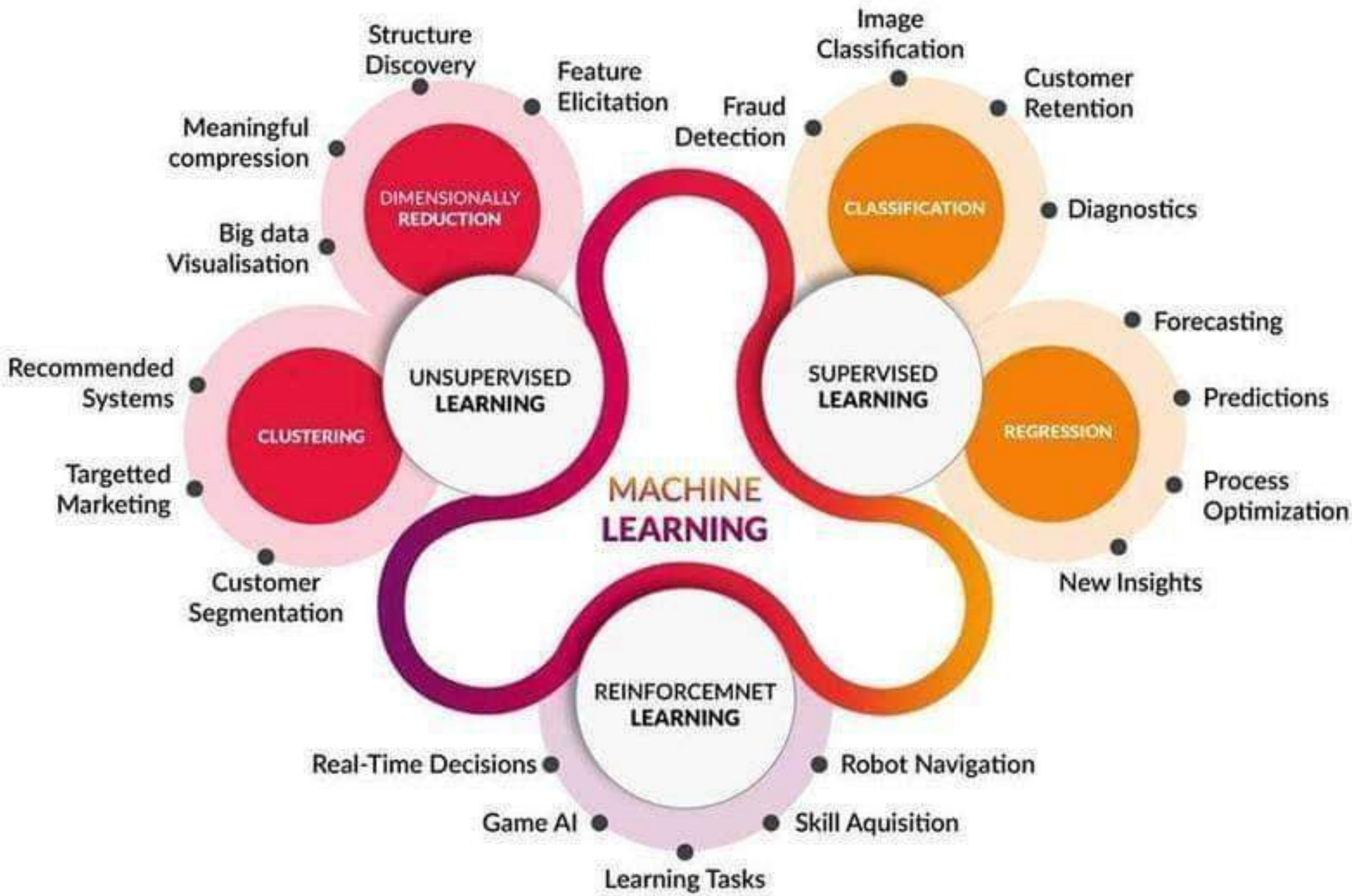
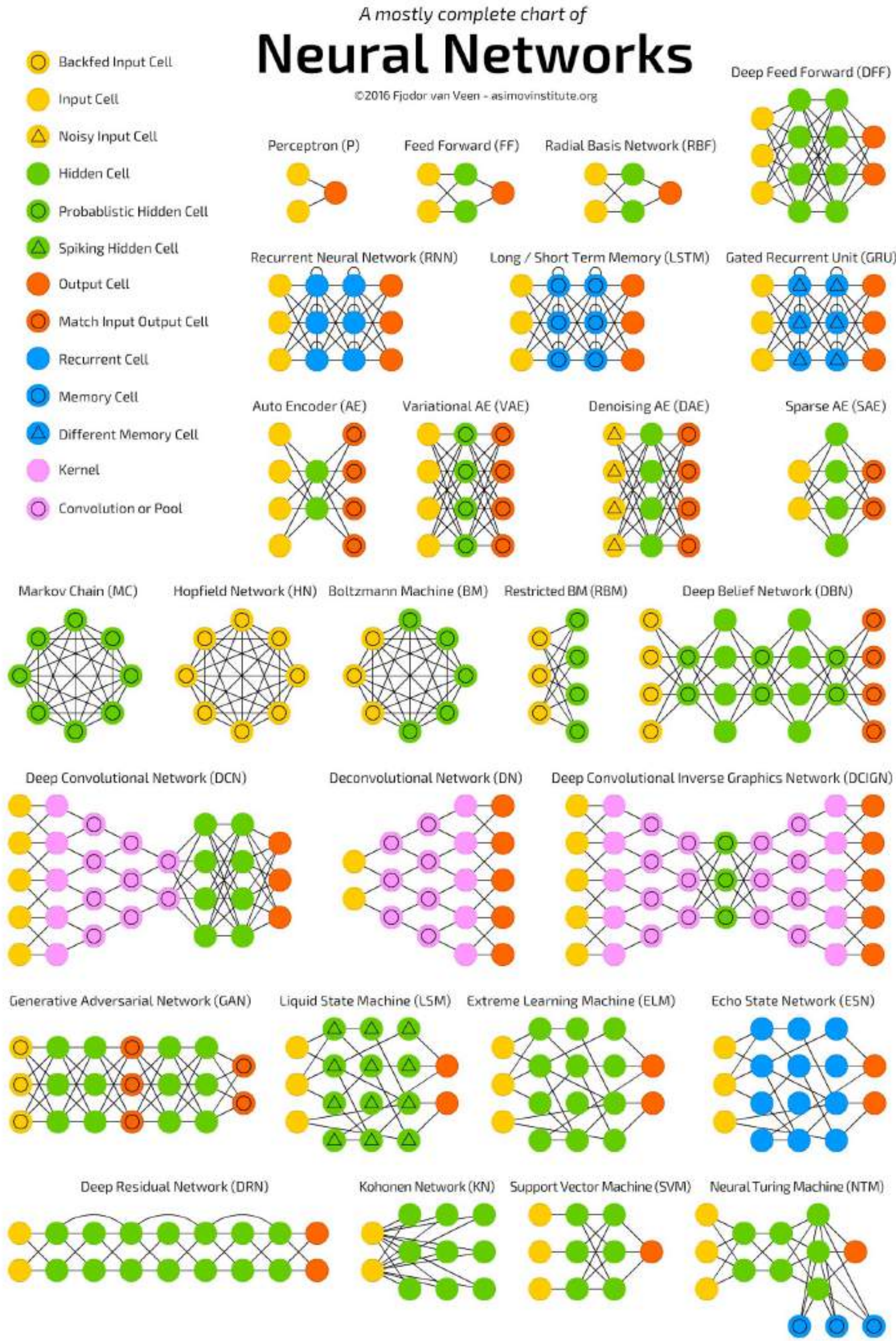
Artificial Neural Networks – I

Manmeet Singh



MACHINE LEARNING
UNSUPERVISED LEARNING
DIMENSIONALLY REDUCTION
Structure Discovery
Feature Elicitation
Meaningful compression
Big data Visualisation
CLUSTERING
Recommended Systems
Targetted Marketing
Customer Segmentation
SUPERVISED LEARNING
CLASSIFICATION
Image Classification
Customer Retention
Fraud Detection
Diagnostics
REGRESSION
Forecasting
Predictions
Process Optimization
New Insights
REINFORCEMNET LEARNING
Real-Time Decisions
Robot Navigation
Game AI
Skill Aquisition
Learning Tasks


A mostly complete chart of
Neural Networks
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Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)
Markov Chain (MC)
Hopfield Network (HN)
Boltzmann Machine (BM)
Restricted BM (RBM)
Deep Belief Network (DBN)
Deep Convolutional Network (DCN)
Deconvolutional Network (DN)
Deep Convolutional Inverse Graphics Network (DCIGN)
Generative Adversarial Network (GAN)
Liquid State Machine (LSM)
Extreme Learning Machine (ELM)
Echo State Network (ESN)
Deep Residual Network (DRN)
Kohonen Network (KN)
Support Vector Machine (SVM)
Neural Turing Machine (NTM)

Machine Learning

- Grew out of work in AI
- New capability for computers

Examples:

- Database mining

    Large datasets from growth of automation/web.

    E.g., Web click data, medical records, biology, engineering
- Applications can’t program by hand.

    E.g., Autonomous helicopter, handwriting recognition, most of Natural Language Processing (NLP), Computer Vision.
- Self-customizing programs

    E.g., Amazon, Netflix product recommendations
- Understanding human learning (brain, real AI).

Machine Learning definition

- Arthur Samuel (1959). Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.
- Tom Mitchell (1998) Well-posed Learning Problem: A computer program is said to *learn* from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.

Machine learning algorithms:

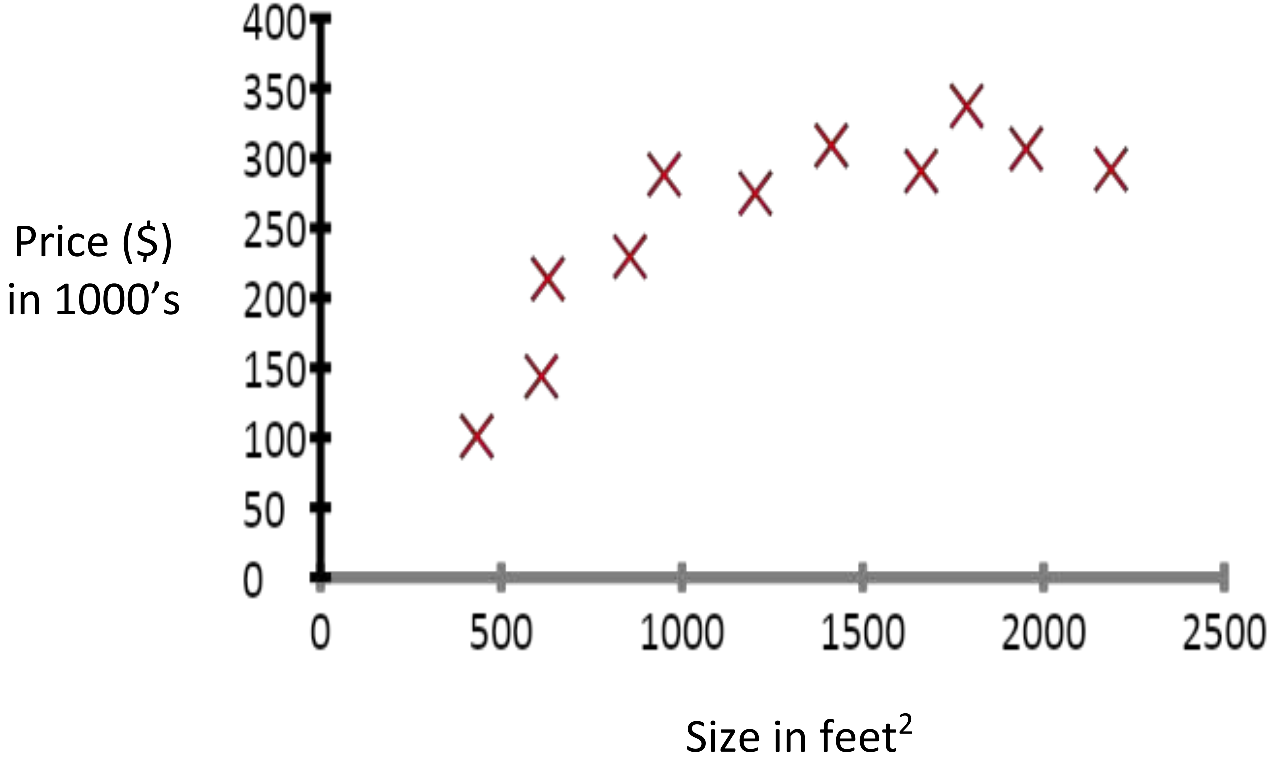
- Supervised learning
- Unsupervised learning

Others: Reinforcement learning, recommender systems.

Also talk about: Practical advice for applying learning algorithms.

Supervised Learning

Housing price prediction.

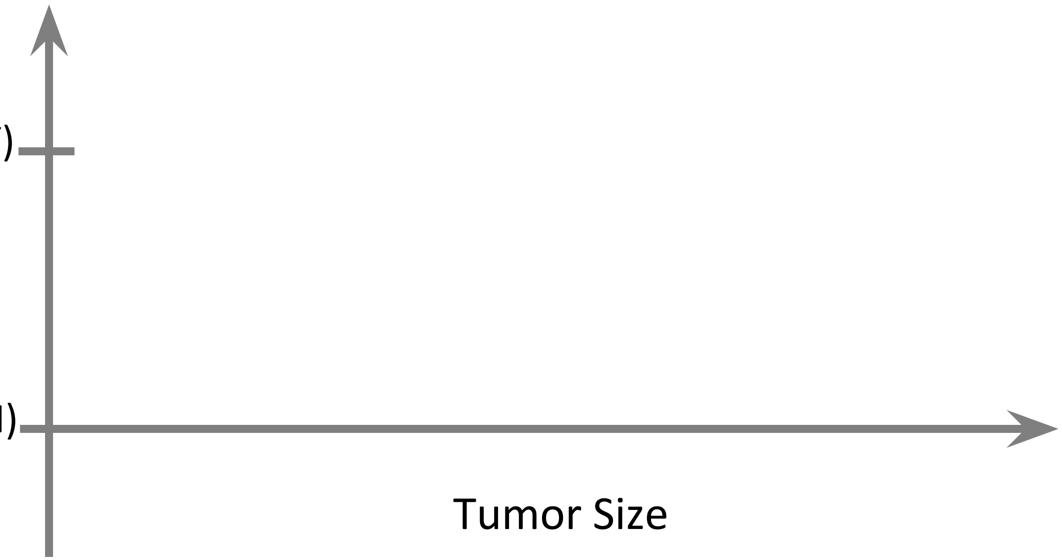


<u>Supervised Learning</u>

"right answers" given

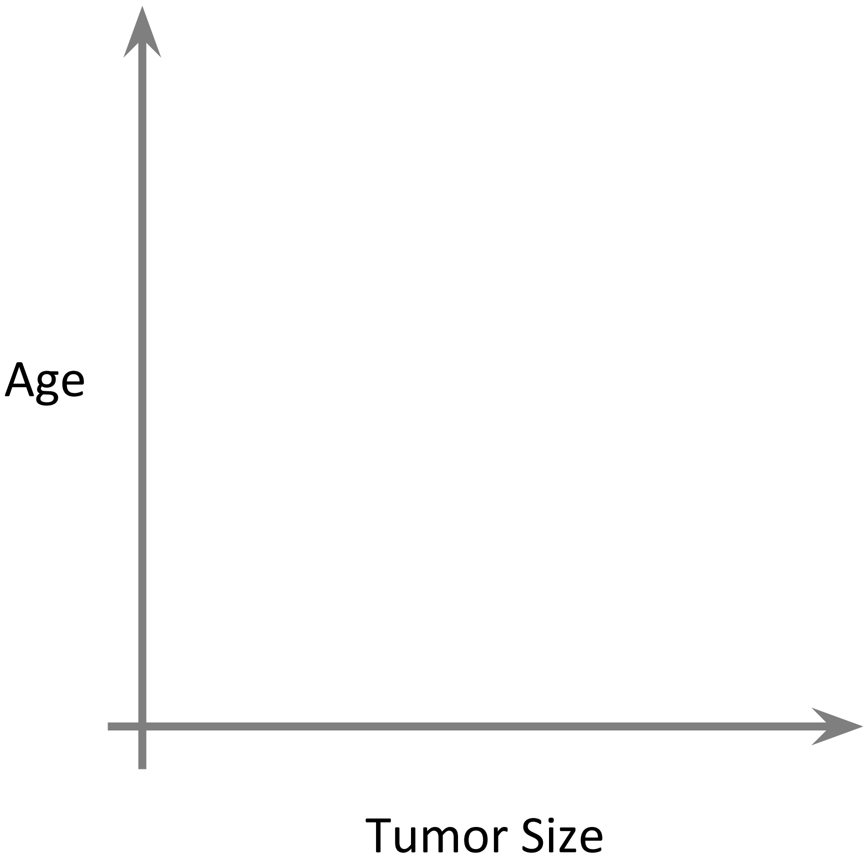
<u>Regression:</u> Predict continuous valued output (price)

Breast cancer (malignant, benign)



<u>Classification</u>

Discrete valued output (0 or 1)



- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape

…

You're running a company, and you want to develop learning algorithms to address each of two problems.

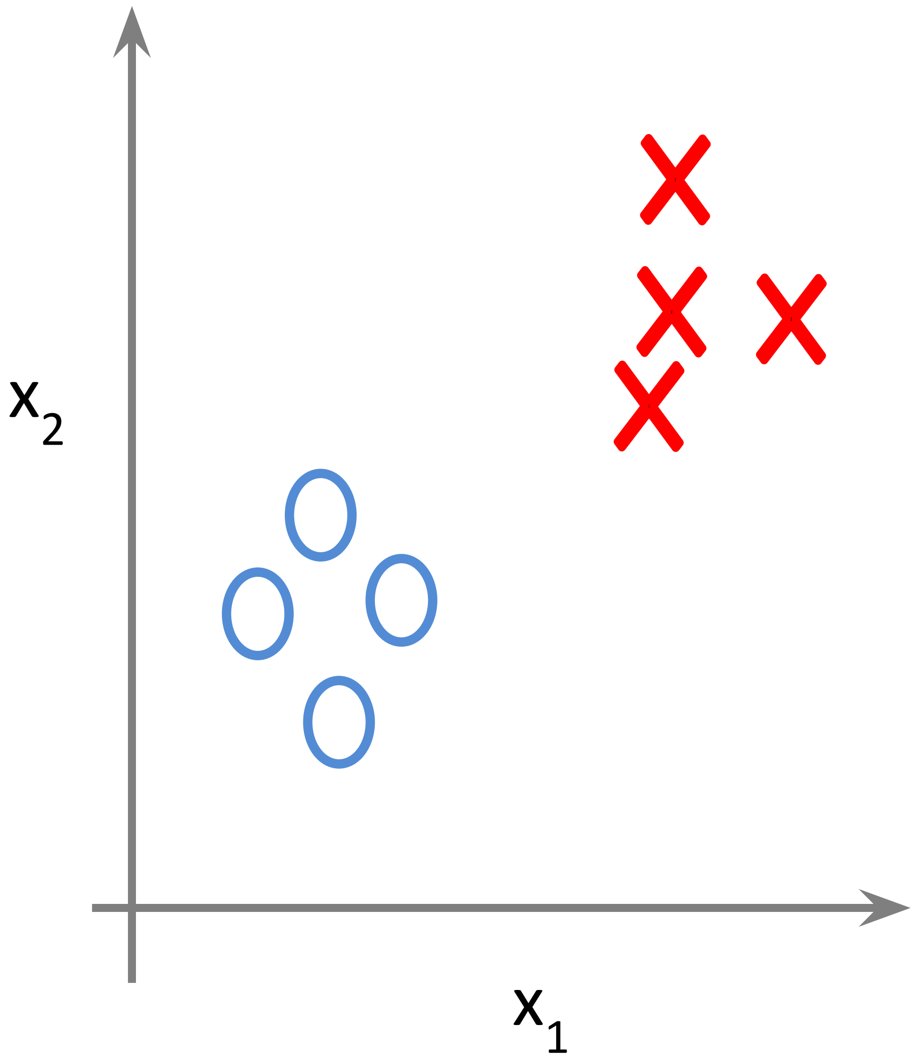
Problem 1: You have a large inventory of identical items. You want to predict how many of these items will sell over the next 3 months.
Problem 2: You'd like software to examine individual customer accounts, and for each account decide if it has been hacked/compromised.

Should you treat these as classification or as regression problems?

- ◯ Treat both as classification problems.
- ◯ Treat problem 1 as a classification problem, problem 2 as a regression problem.
- ◯ Treat problem 1 as a regression problem, problem 2 as a classification problem.
- ◯ Treat both as regression problems.

Unsupervised Learning

Supervised Learning



Unsupervised Learning

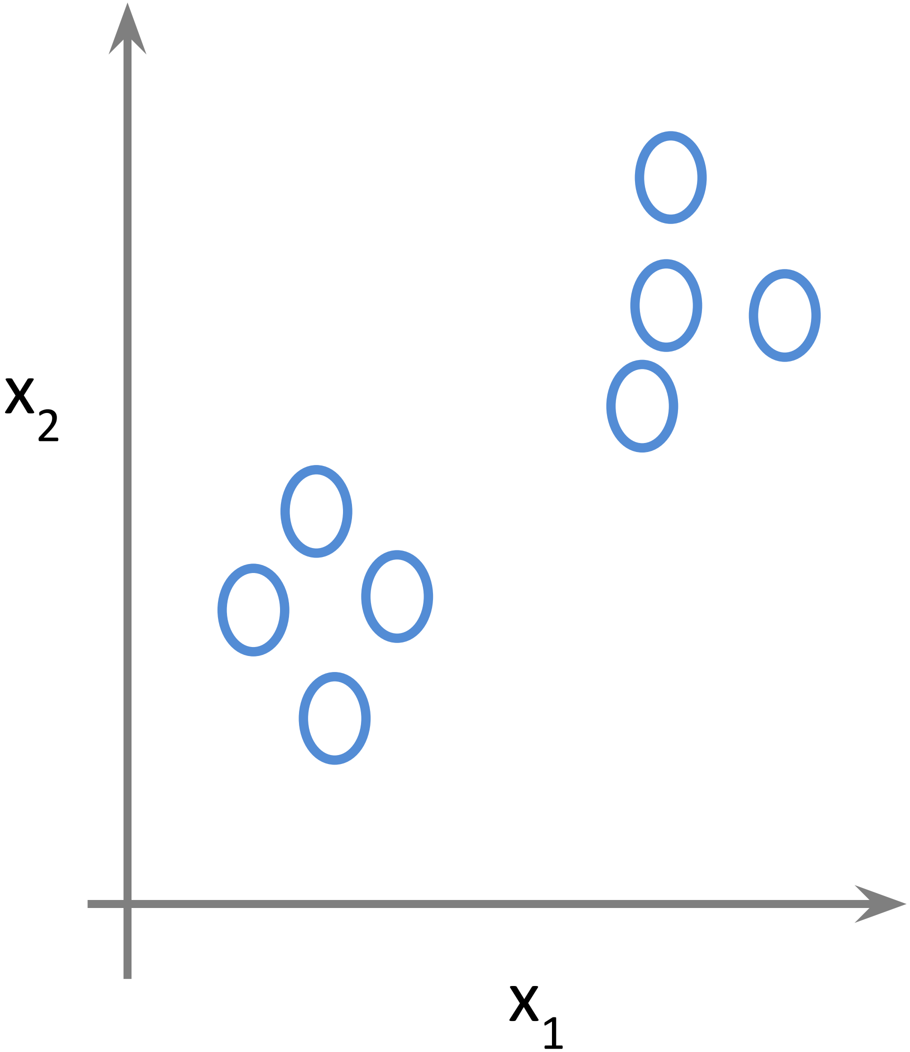
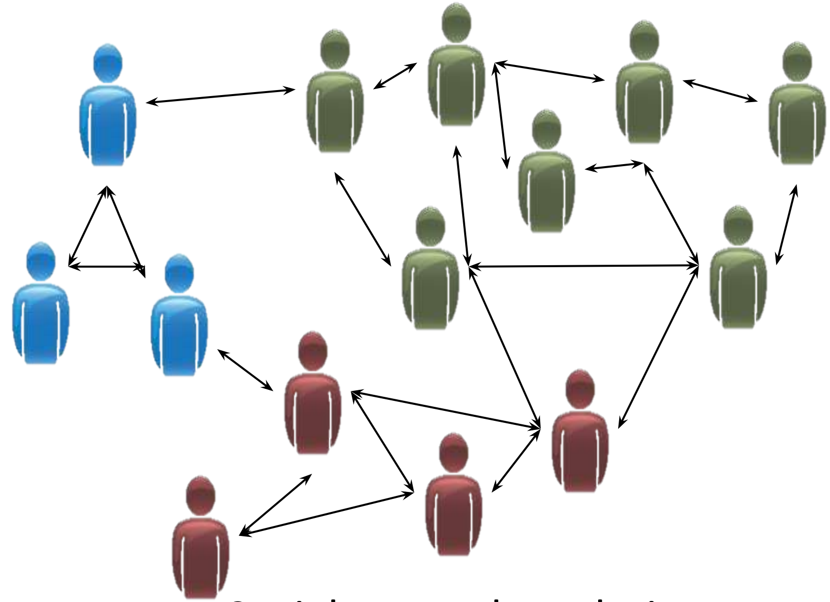
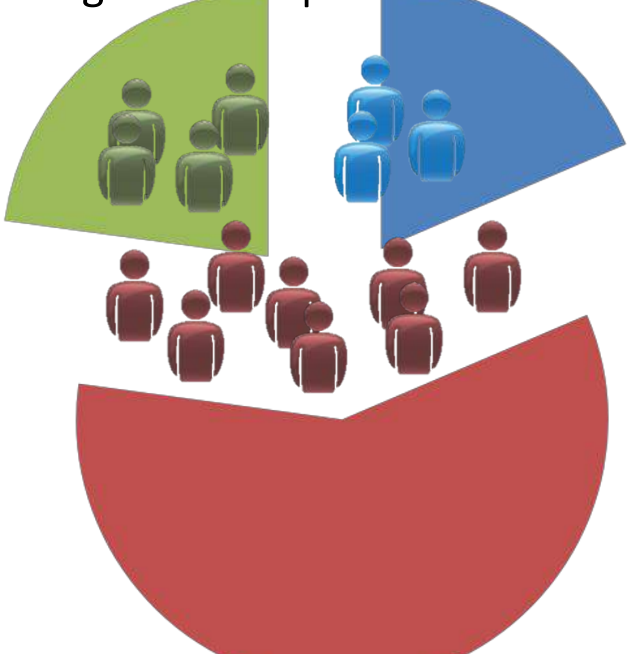


Image credit: NASA/JPL-Caltech/E. Churchwell (Univ. of Wisconsin, Madison)

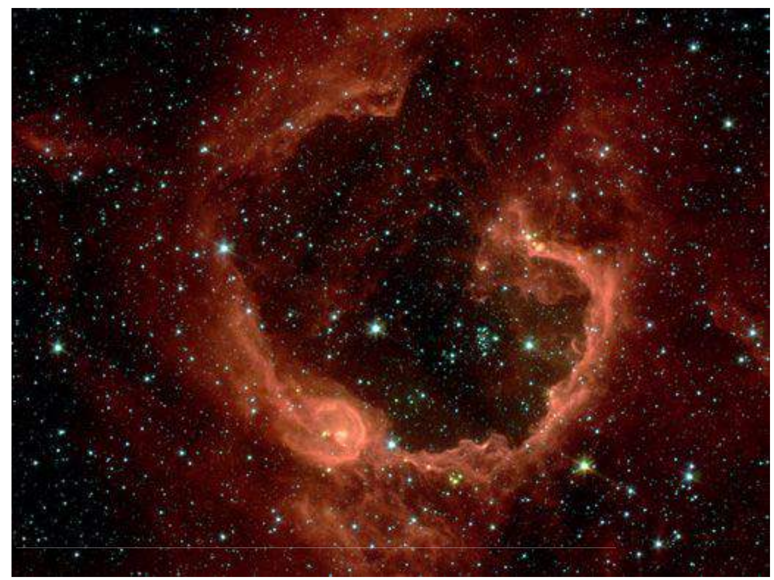
Organize computing clusters



Social network analysis



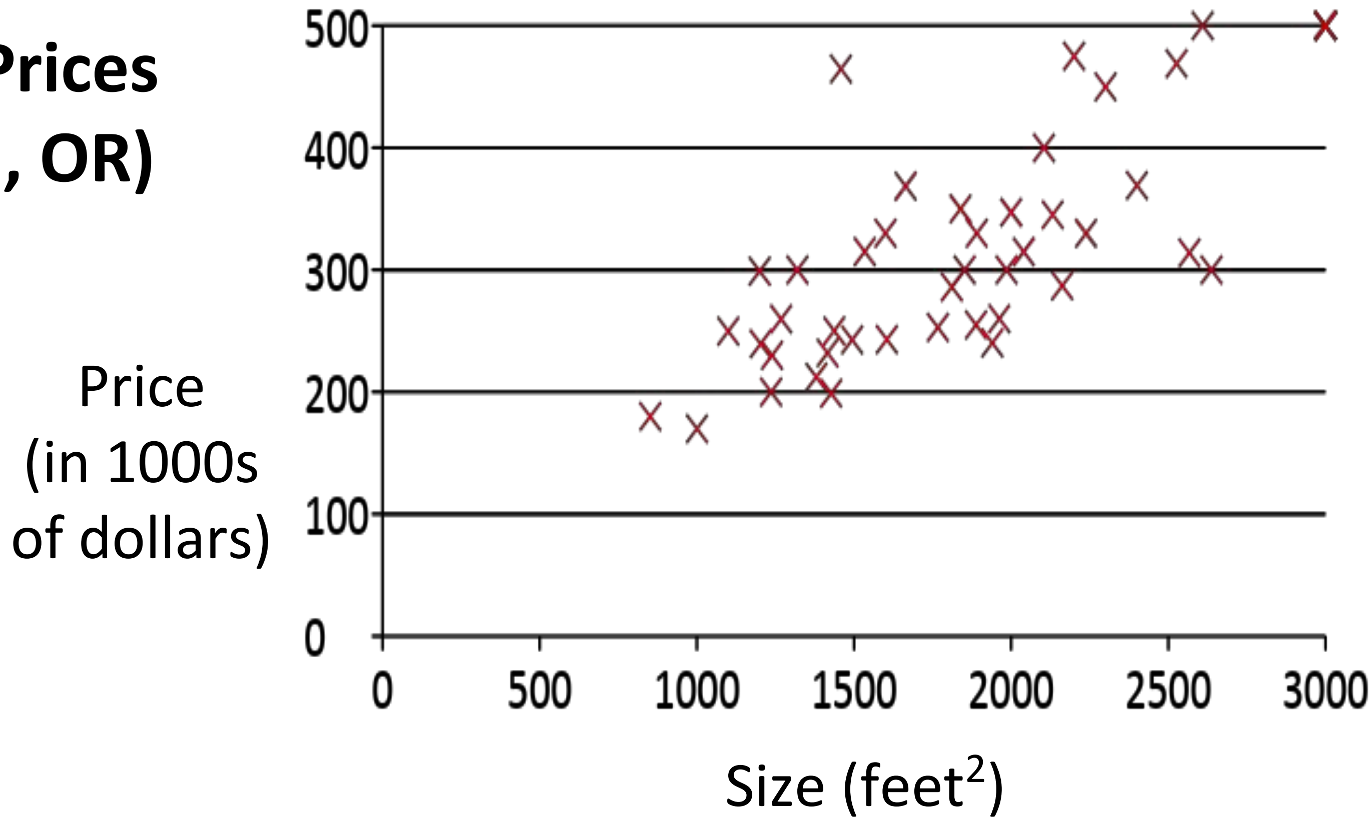
Market segmentation



Astronomical data analysis

Model representation

Housing Prices (Portland, OR)



Supervised Learning

Given the “right answer” for each example in the data.

Regression Problem

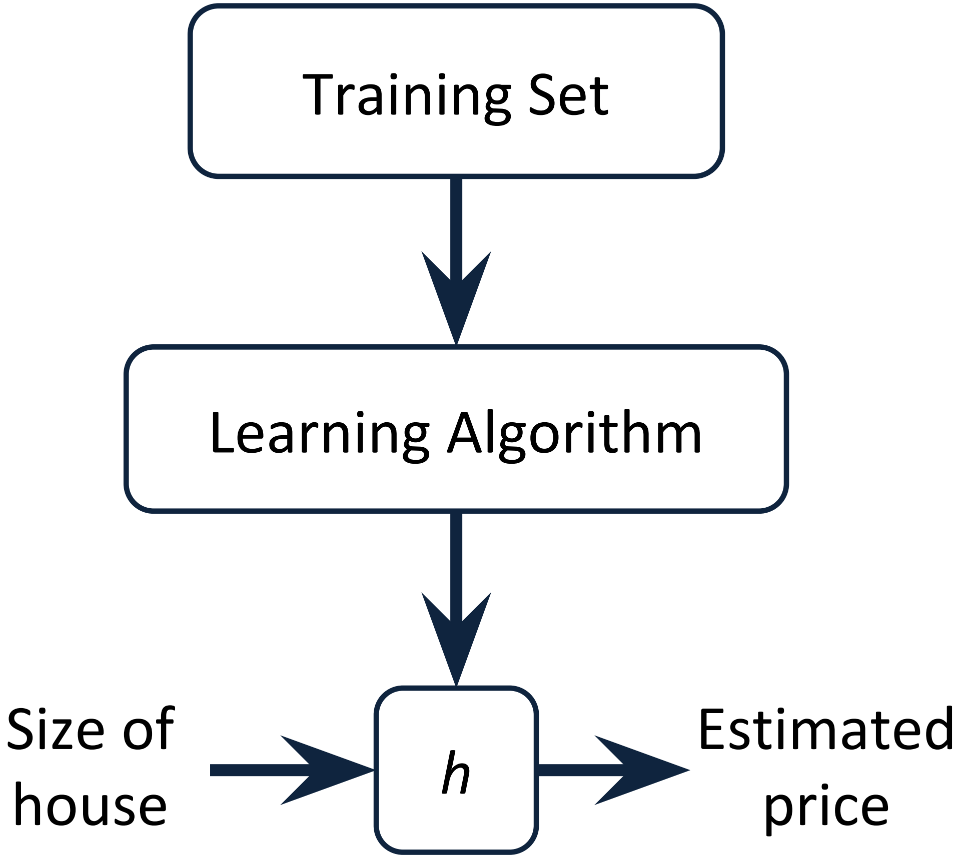
Predict real-valued output

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
…	…

Notation:

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



How do we represent *h* ?

Linear regression with one variable.
Univariate linear regression.

Cost function

Training Set

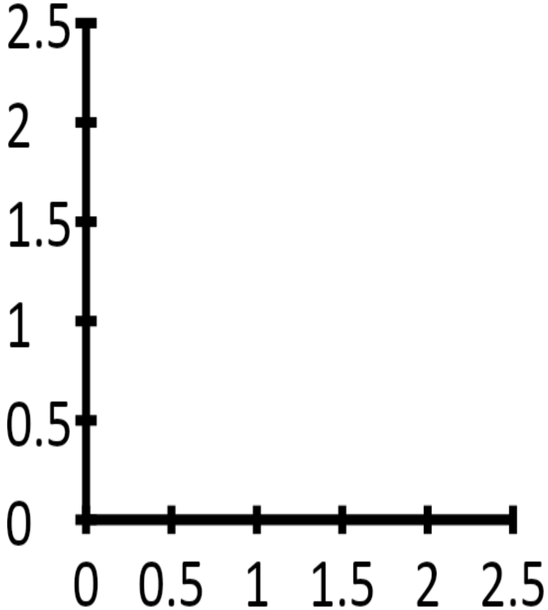
Size in feet^2 (x)	**Price ($) in 1000's (y)**
2104	460
1416	232
1534	315
852	178
…	…

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

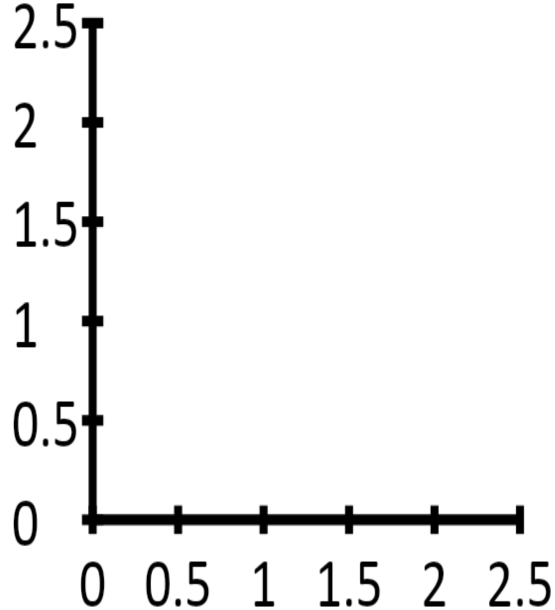
θ_i's: Parameters

How to choose θ_i's ?

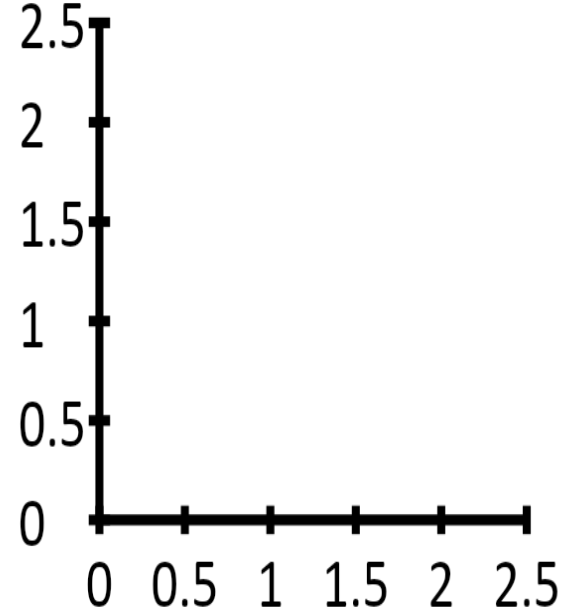
$$h_\theta(x) = \theta_0 + \theta_1 x$$



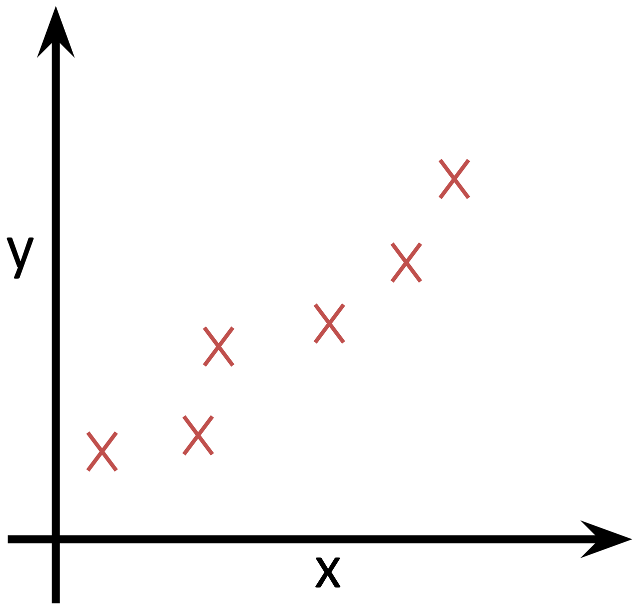
$\theta_0 = 1.5$
$\theta_1 = 0$



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



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



Idea: Choose θ_0, θ_1 so that

$h_\theta(x)$ is close to y for our training examples (x, y)

Hypothesis:

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

Parameters:

$$\theta_0, \theta_1$$

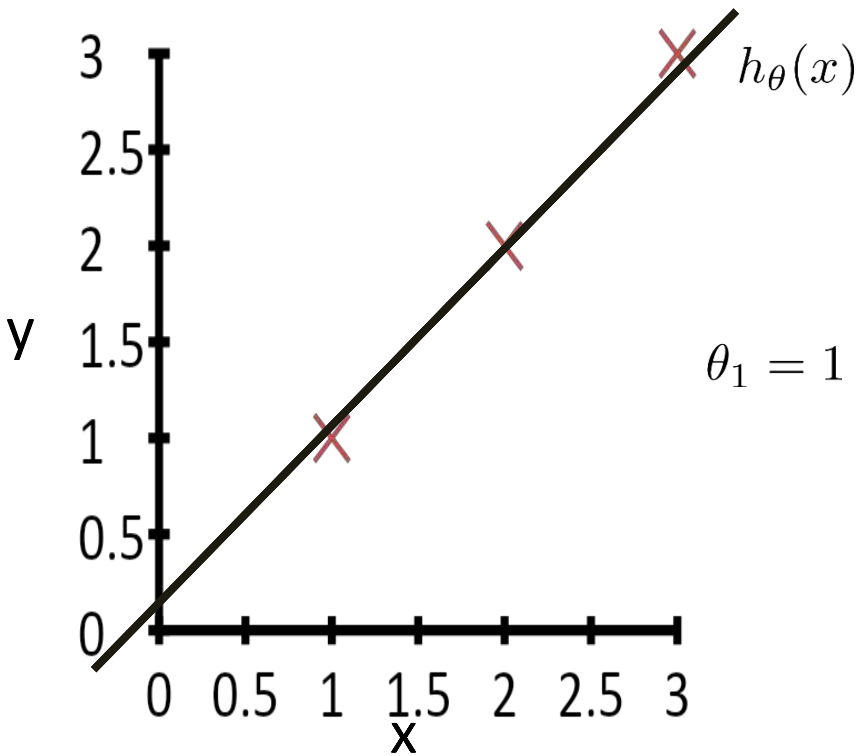
Cost Function:

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

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

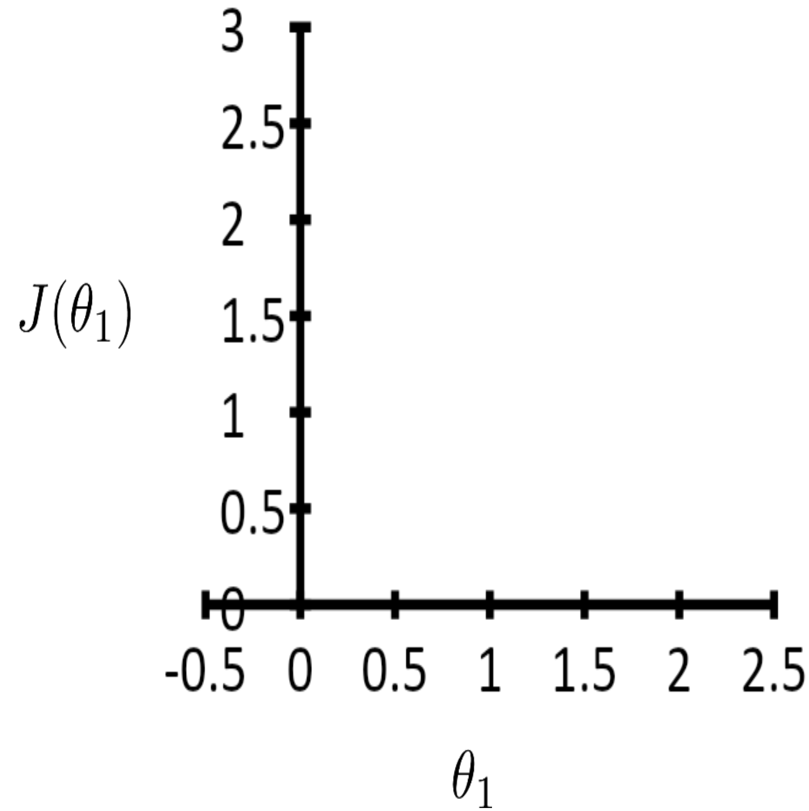
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



$h_\theta(x)$

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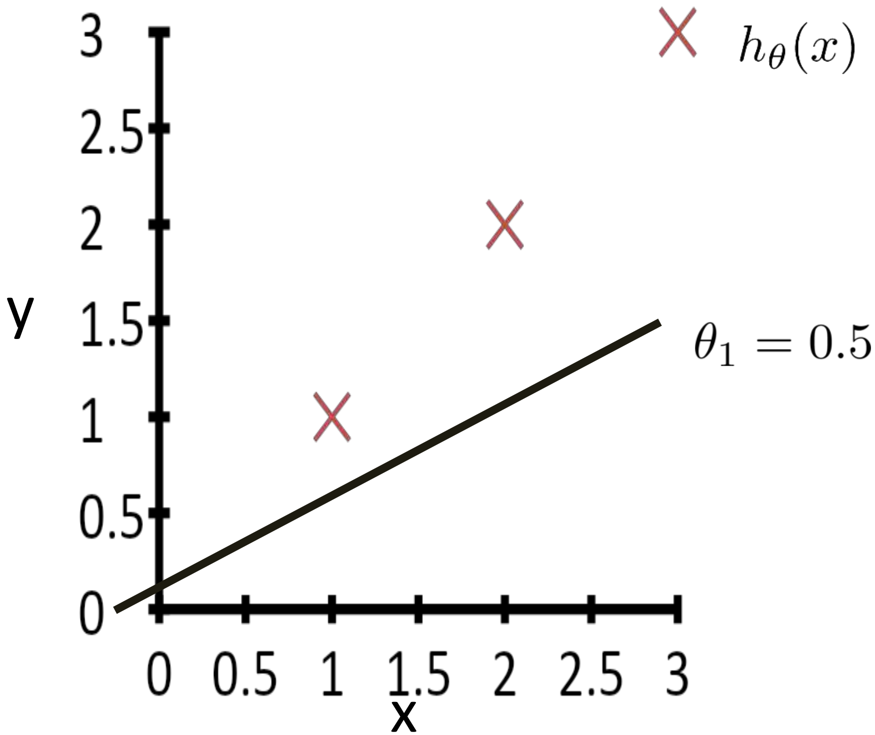

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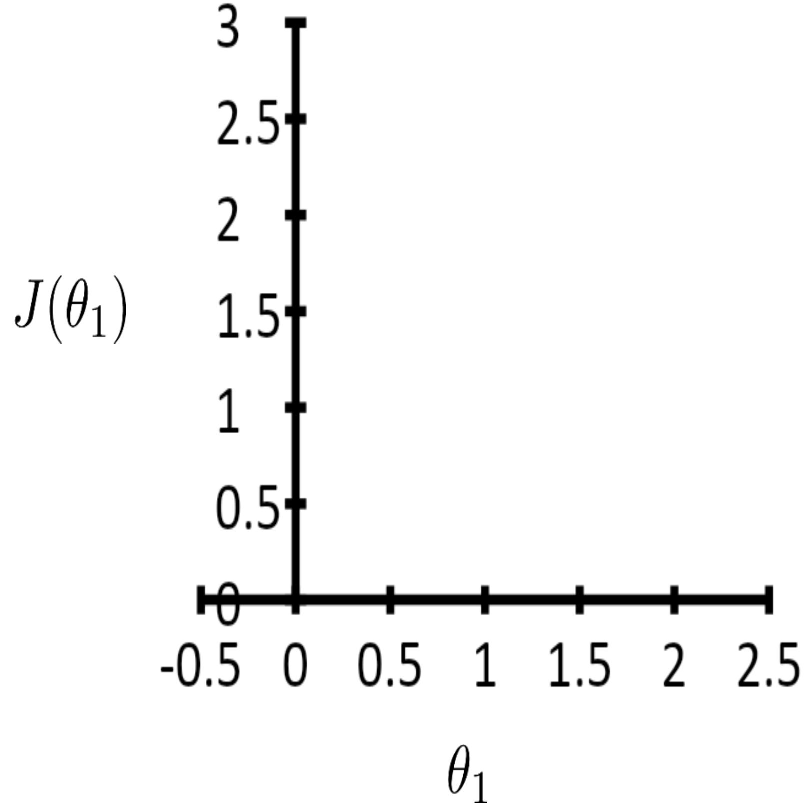

$h_\theta(x)$

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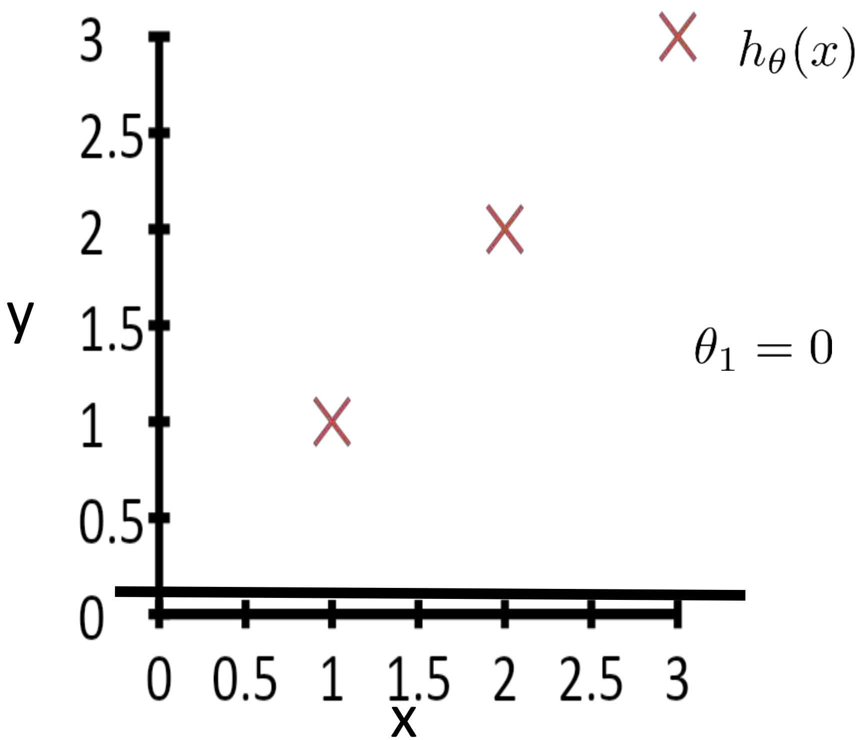

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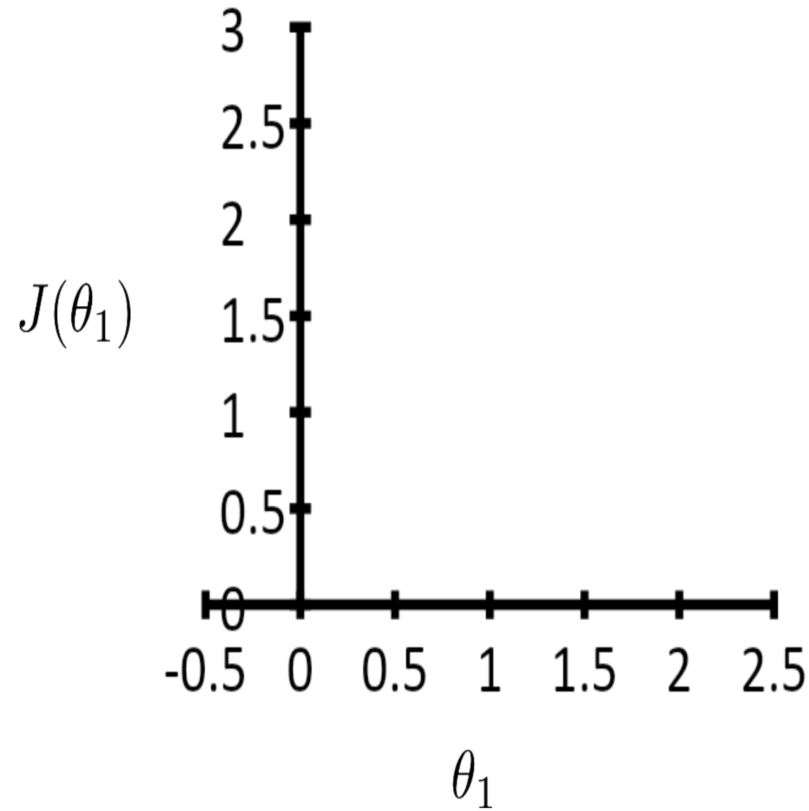


Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x$

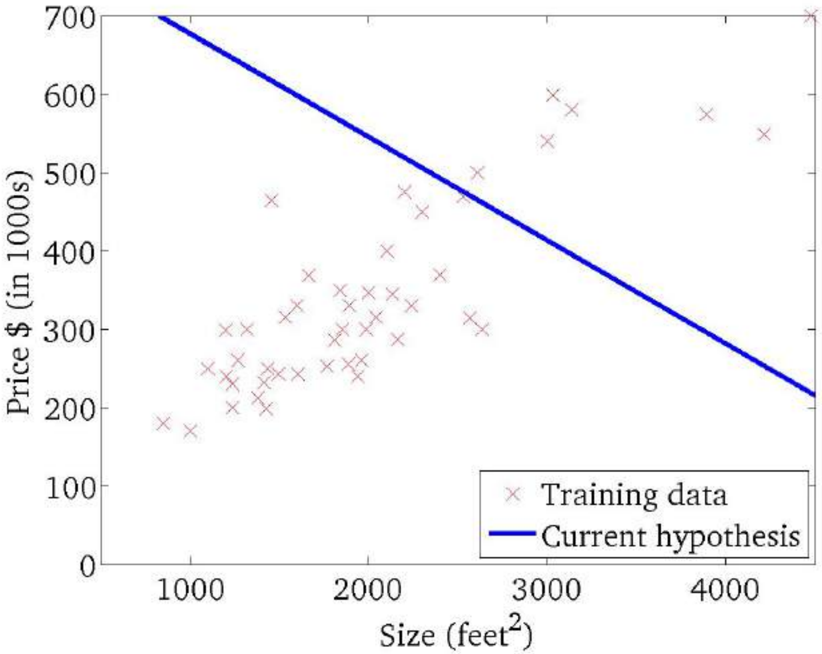
Parameters: θ_0, θ_1

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

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

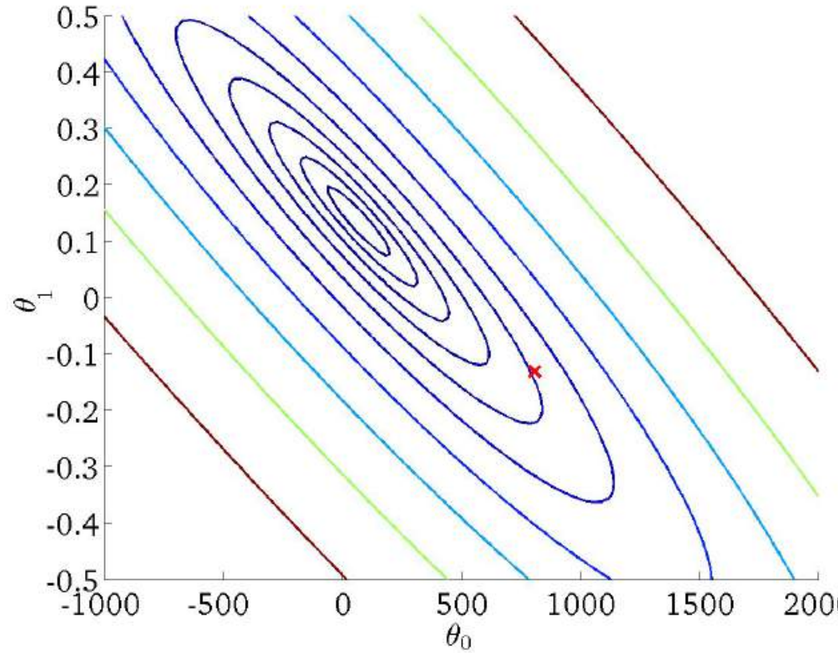
$$h_\theta(x)$$

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



$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



$h_\theta(x)$

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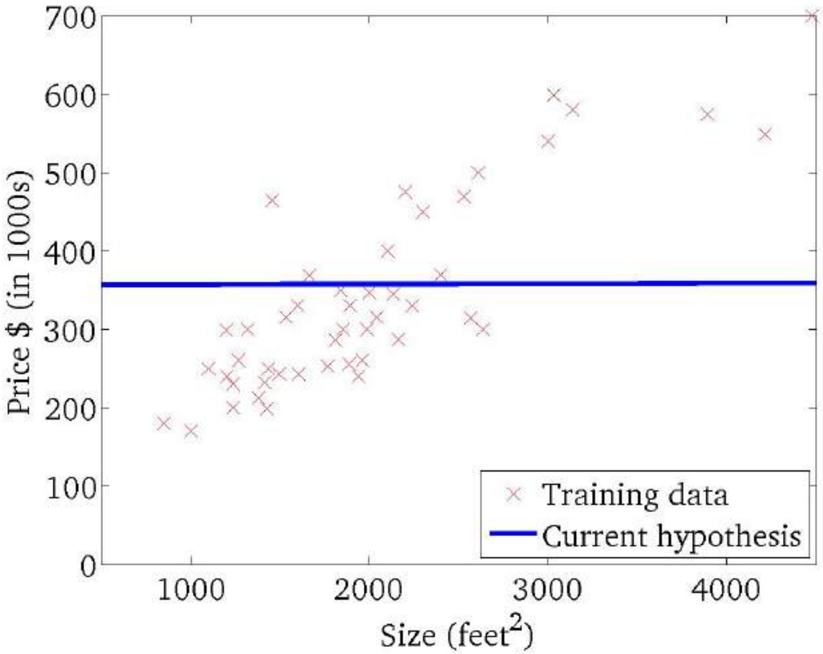

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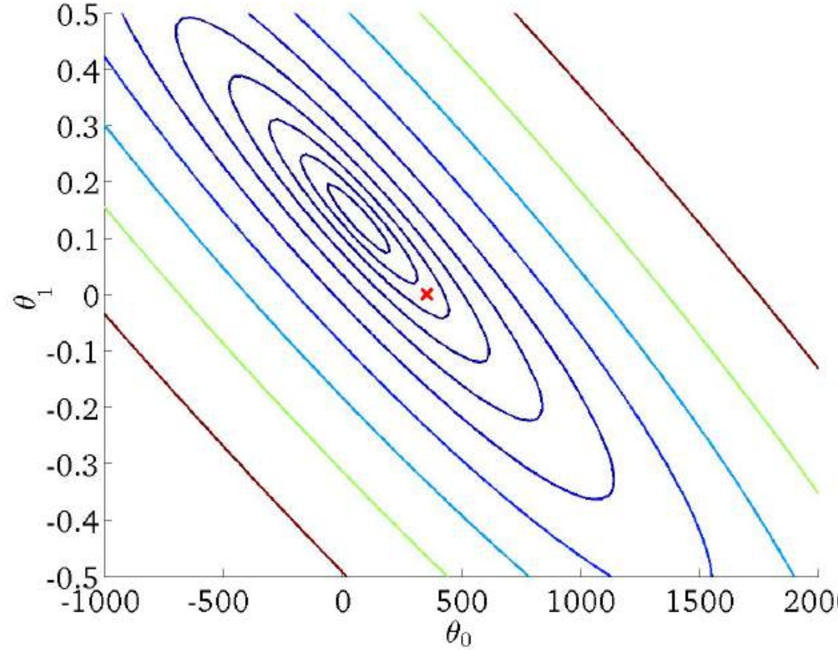

$$h_\theta(x)$$

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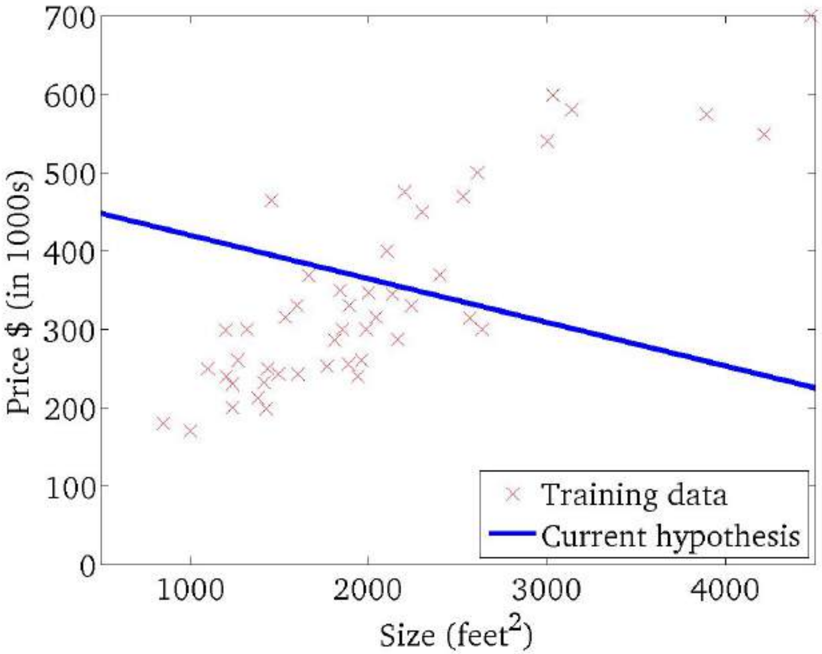
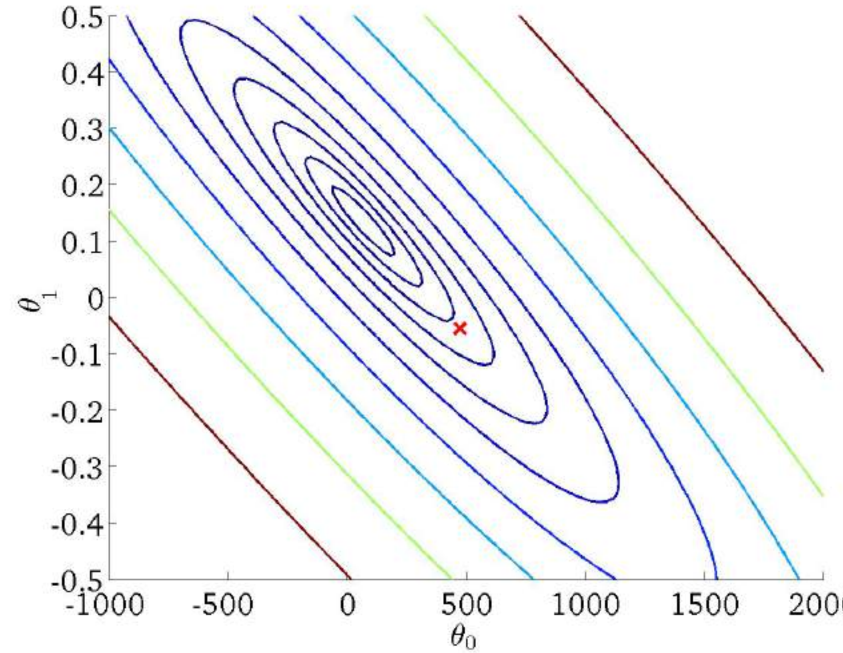


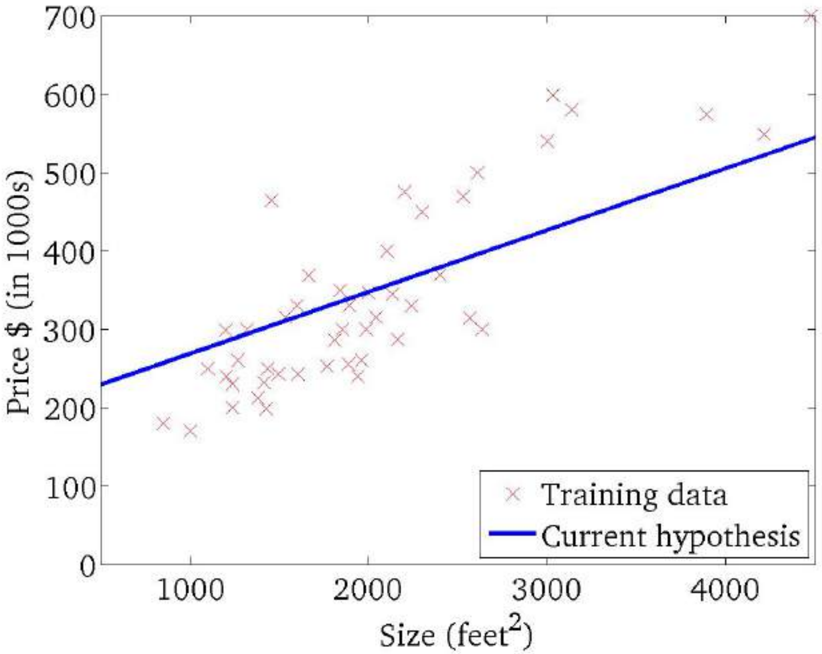
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



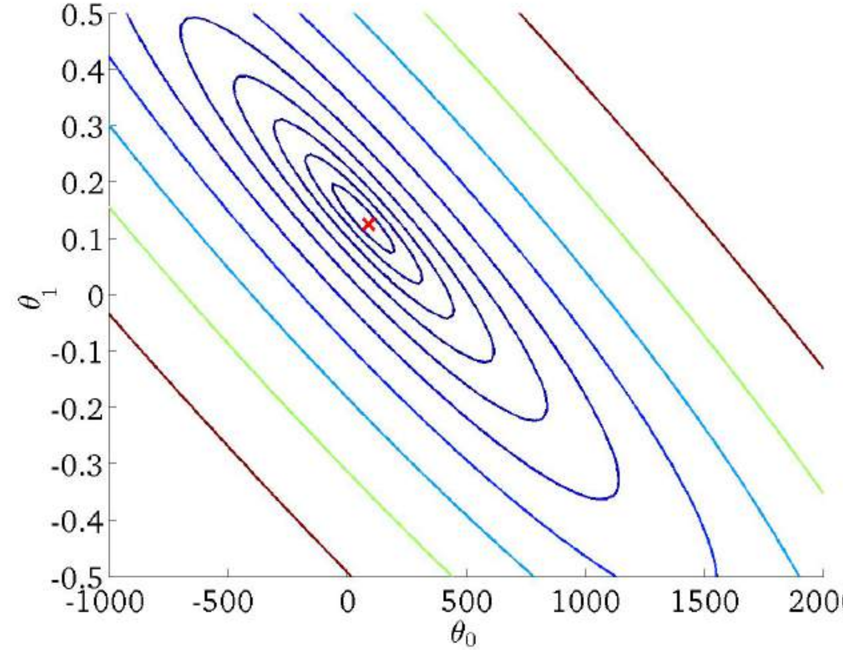
$h_\theta(x)$

(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

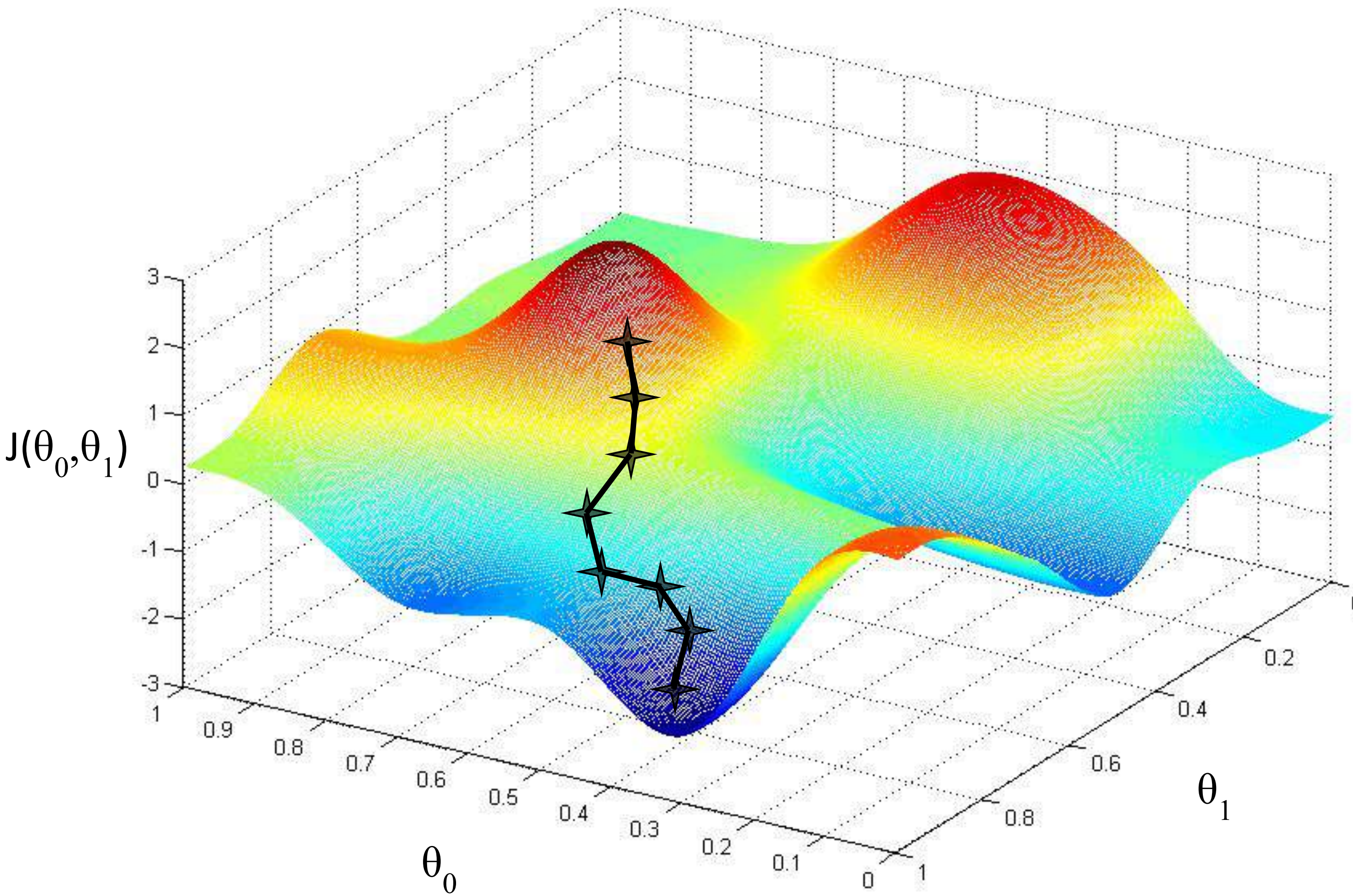
Have some function $J(\theta_0, \theta_1)$

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

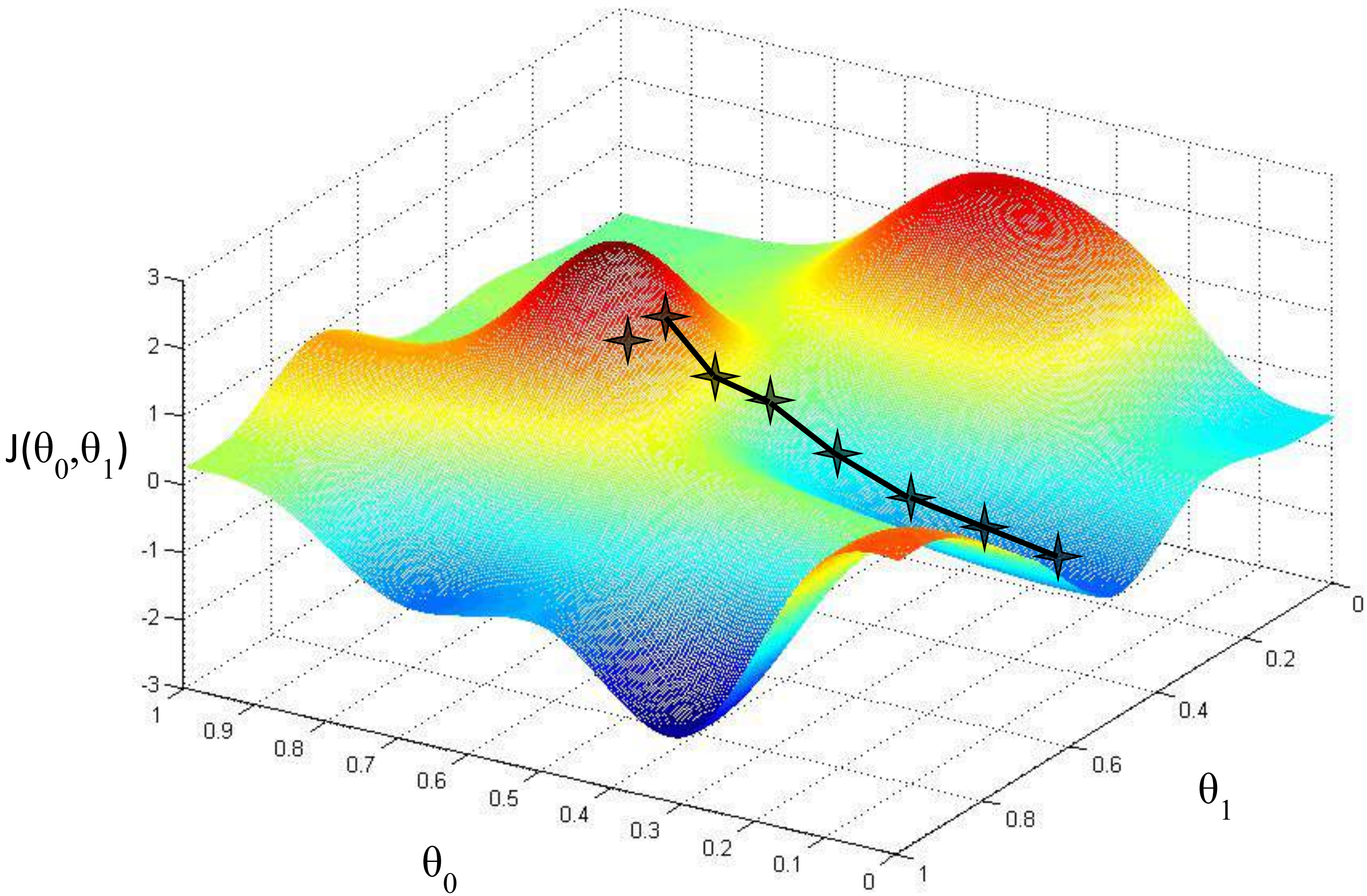
Outline:

- Start with some
- 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
J(θ0,θ1)
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

Gradient descent algorithm

$$
\begin{aligned}
&\text{repeat until convergence } \{ \\
&\quad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad (\text{for } j = 0 \text{ and } j = 1) \\
&\}
\end{aligned}
$$

Correct: Simultaneous update

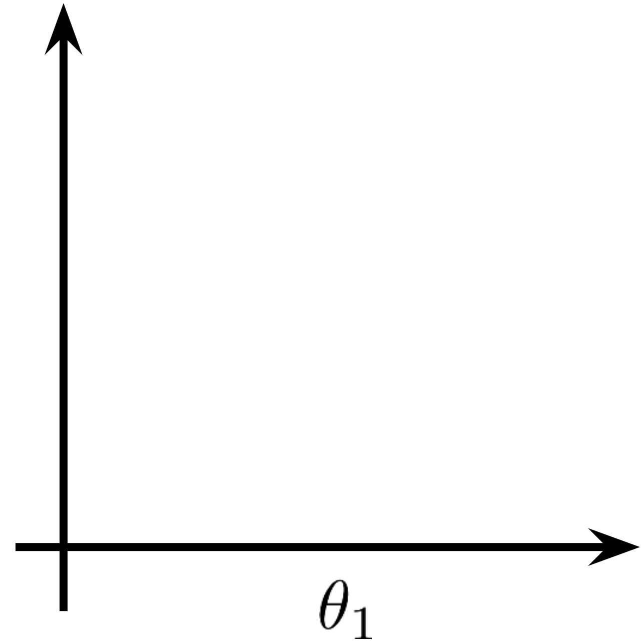
$$
\begin{aligned}
&\text{temp0} := \theta_0 - \alpha \tfrac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\
&\text{temp1} := \theta_1 - \alpha \tfrac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\
&\theta_0 := \text{temp0} \\
&\theta_1 := \text{temp1}
\end{aligned}
$$

Incorrect:

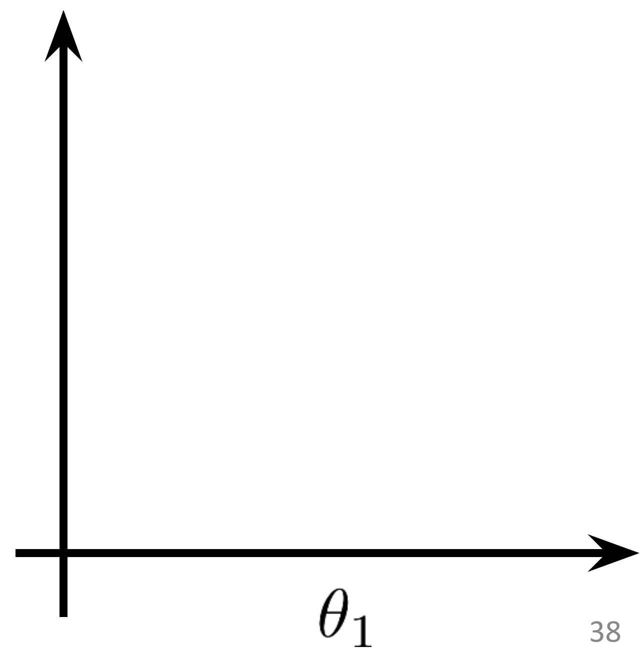
$$
\begin{aligned}
&\text{temp0} := \theta_0 - \alpha \tfrac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\
&\theta_0 := \text{temp0} \\
&\text{temp1} := \theta_1 - \alpha \tfrac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \\
&\theta_1 := \text{temp1}
\end{aligned}
$$

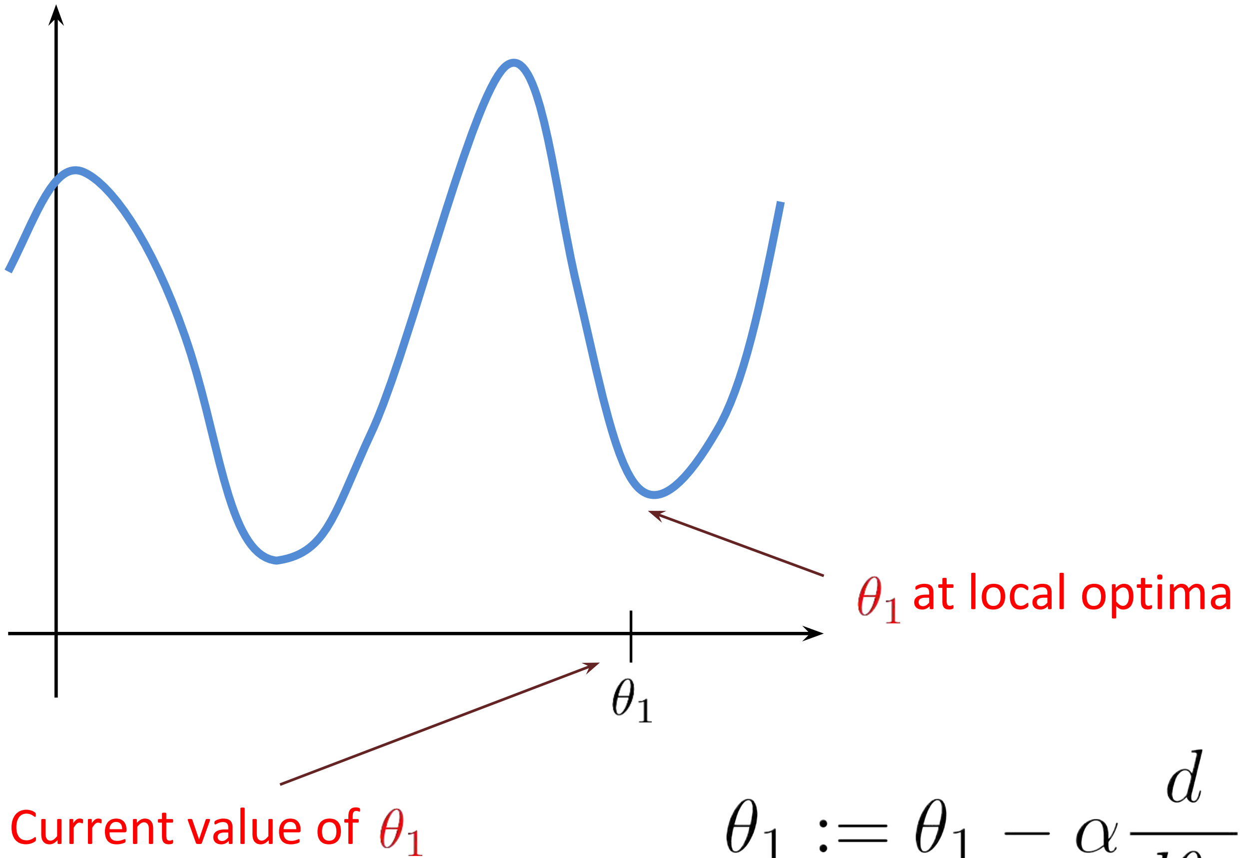
$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

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.



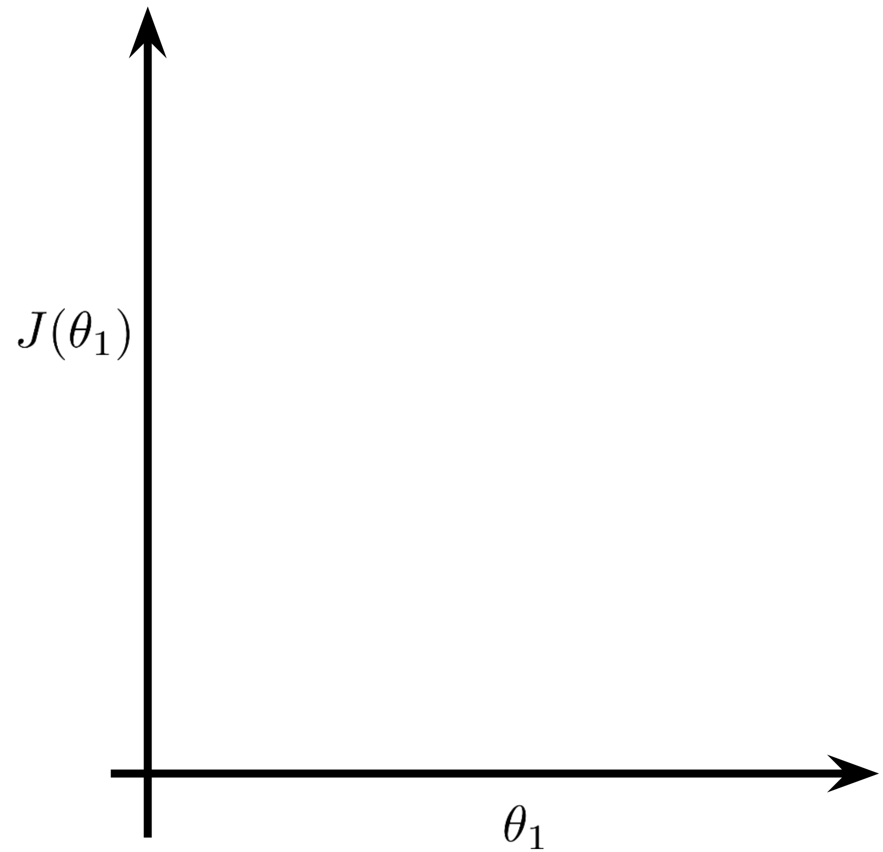


$$\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$$

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 for linear regression

Gradient descent algorithm

$$
\begin{aligned}
&\text{repeat until convergence } \{ \\
&\quad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \\
&\qquad (\text{for } j = 1 \text{ and } j = 0) \\
&\}
\end{aligned}
$$

Linear Regression Model

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

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

Gradient descent algorithm

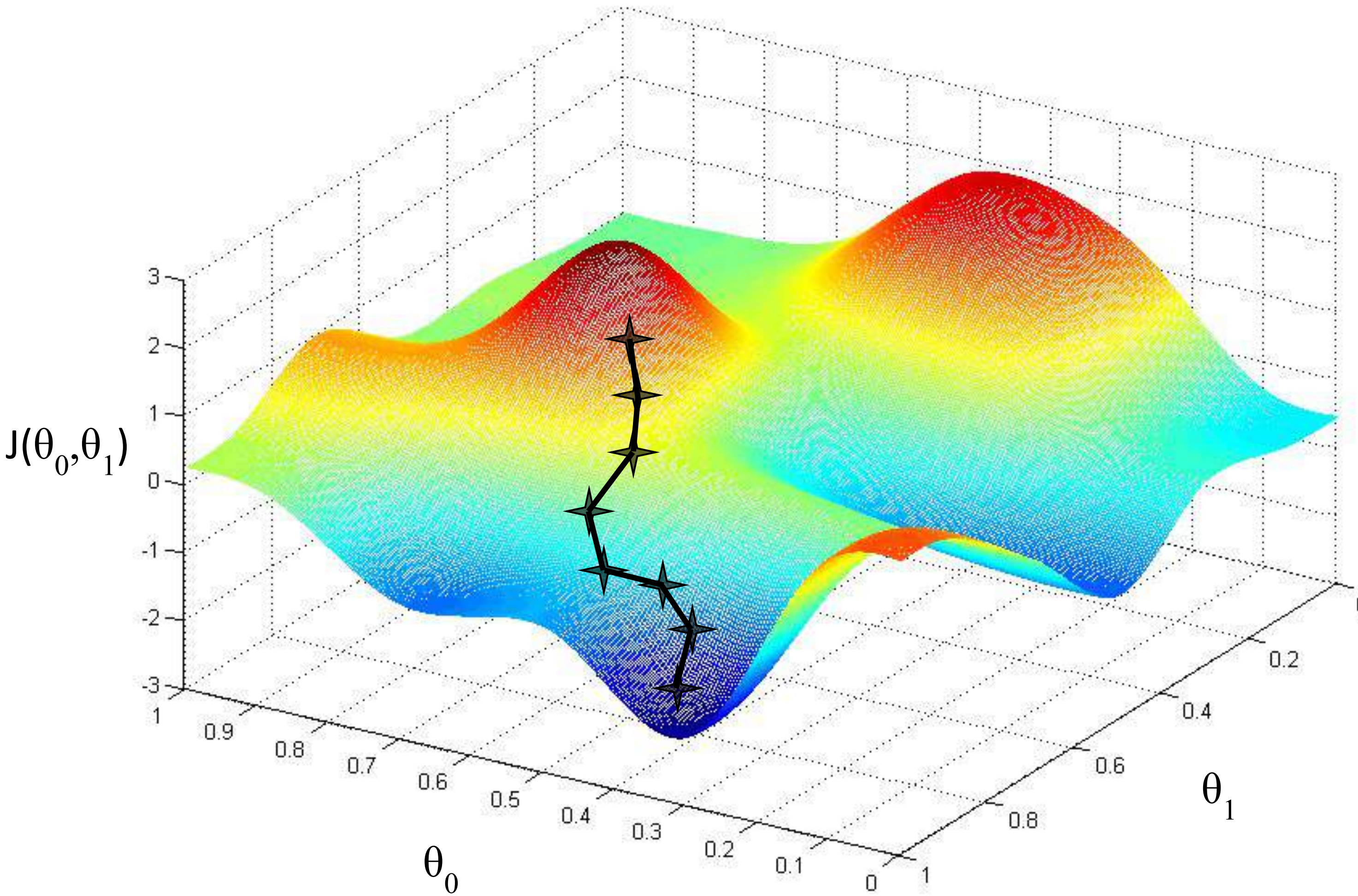
repeat until convergence {

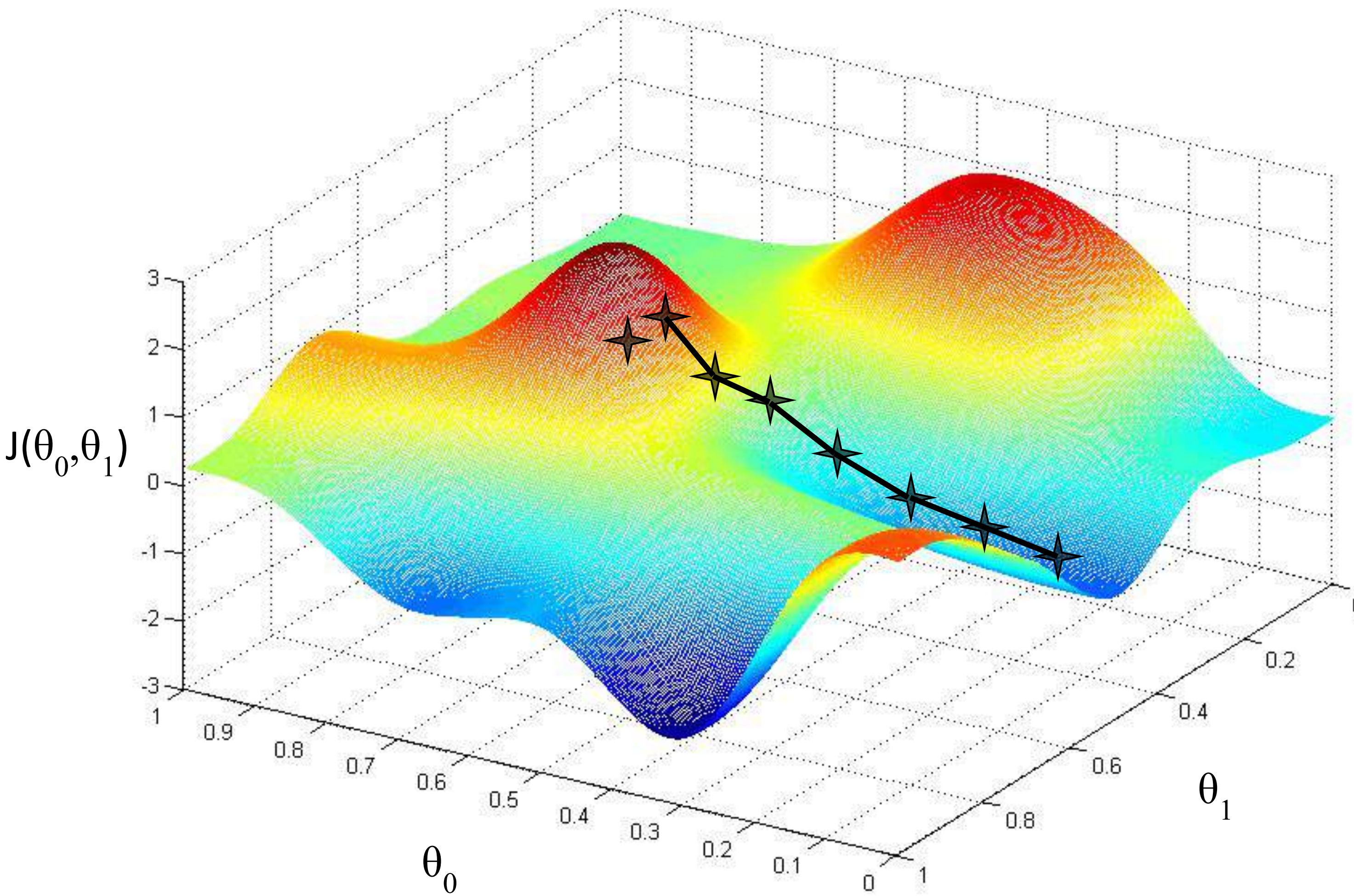
$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)}\right)$$

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

}

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
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0
-1
-2
-3
1
0.9
0.8
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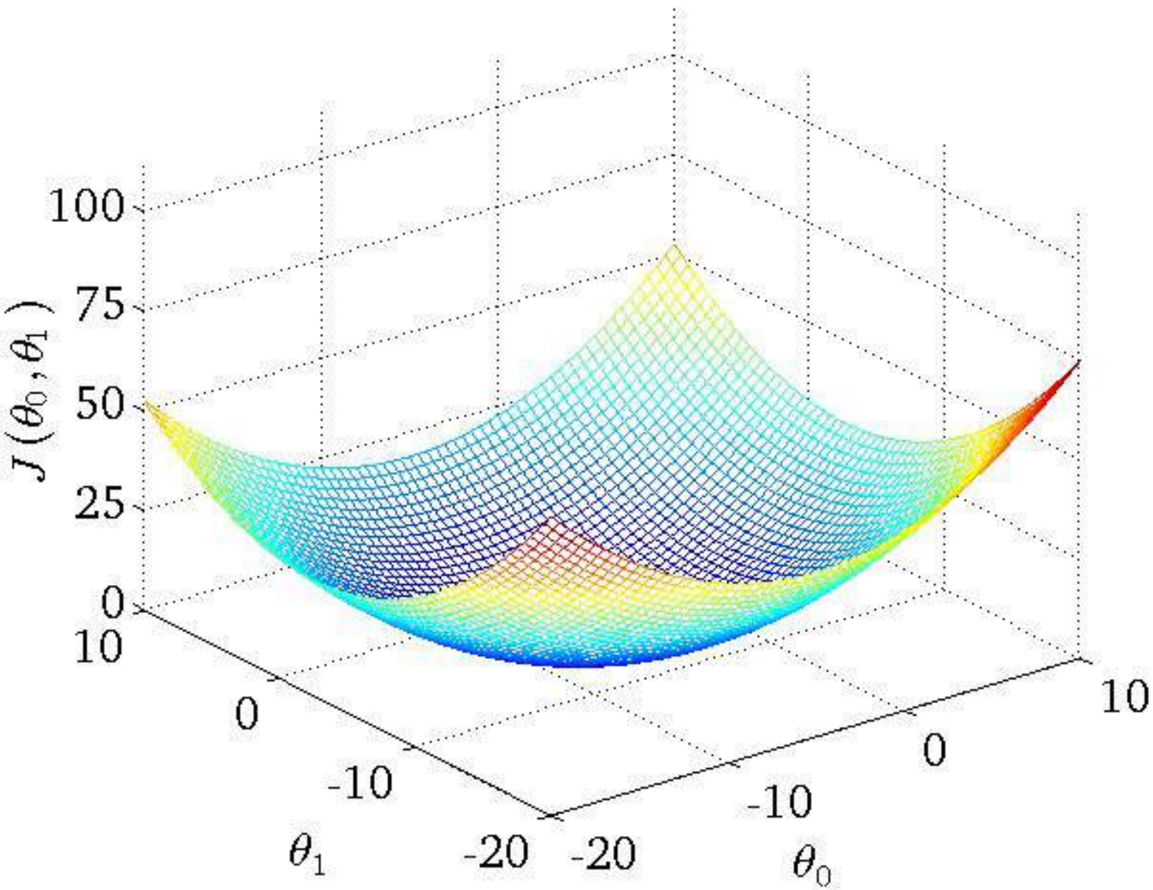
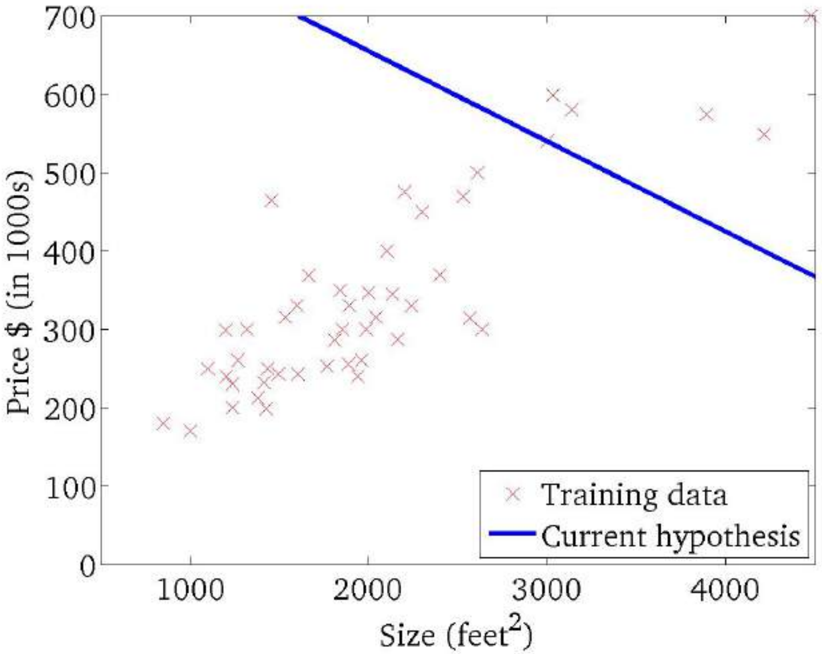
0.5
0.4
0.3
0.2
0.1
0
θ0
0
0.2
0.4
0.6
0.8
1
θ1


100
75
50
25
0
$J(\theta_0, \theta_1)$
10
0
-10
-20
θ_1
-20
-10
0
10
θ_0

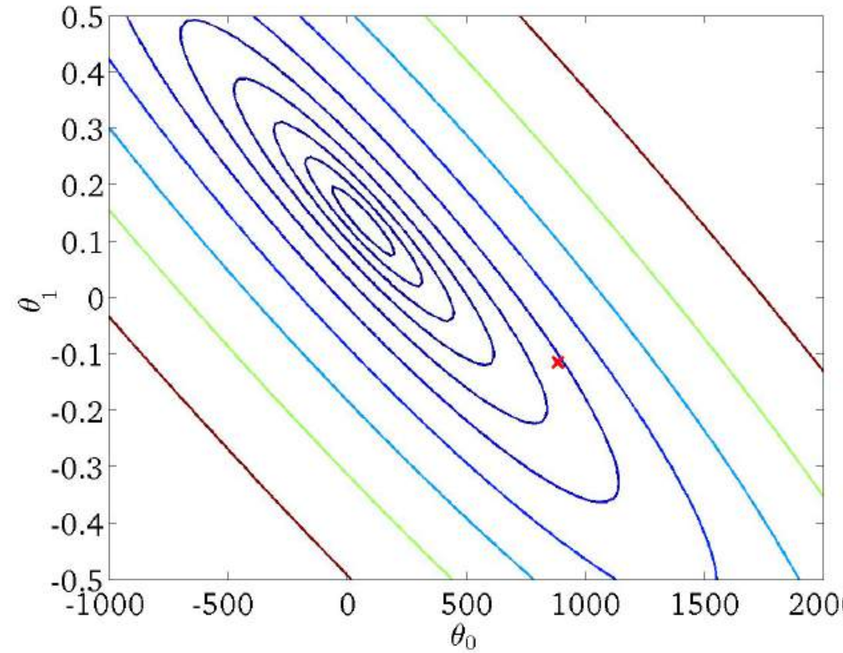
$h_\theta(x)$

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



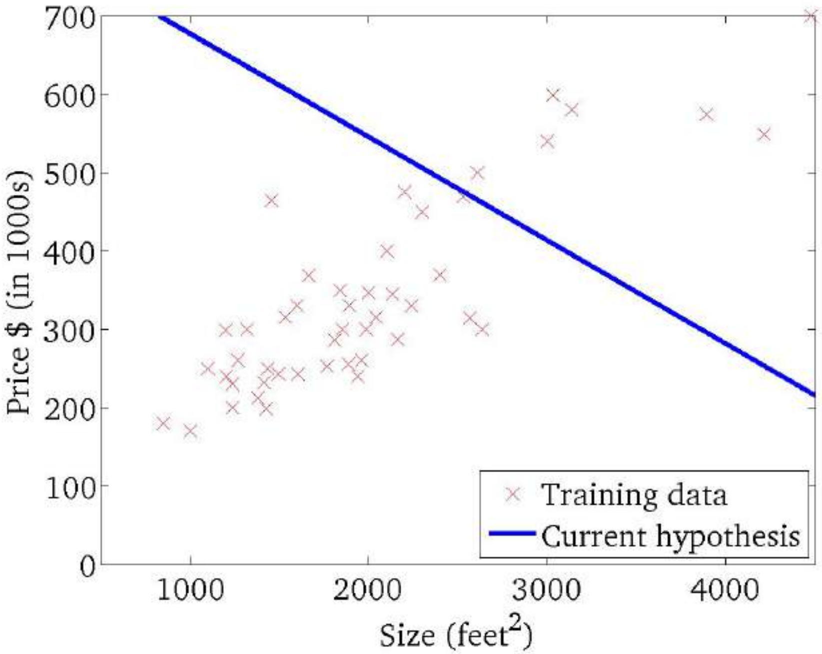
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



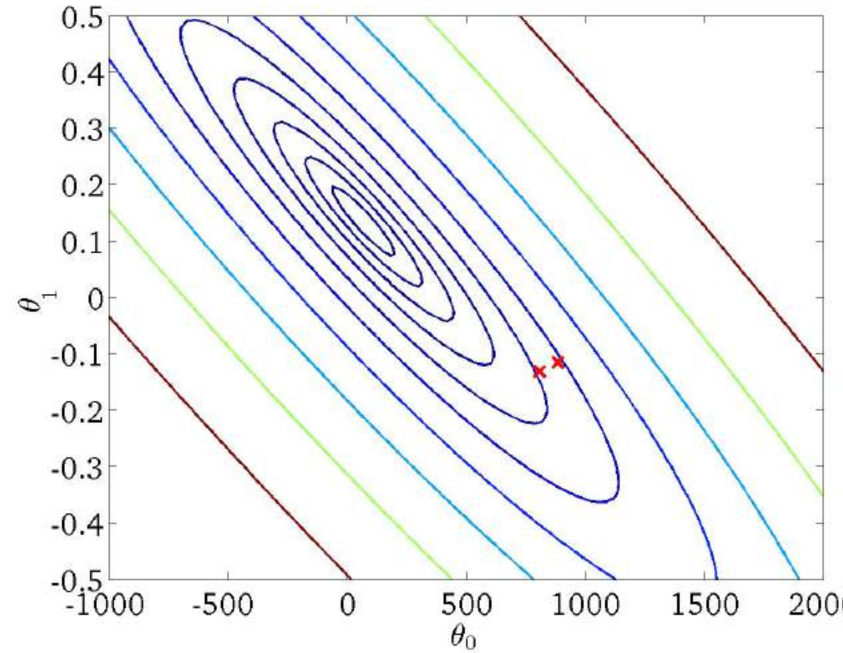
$h_\theta(x)$

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



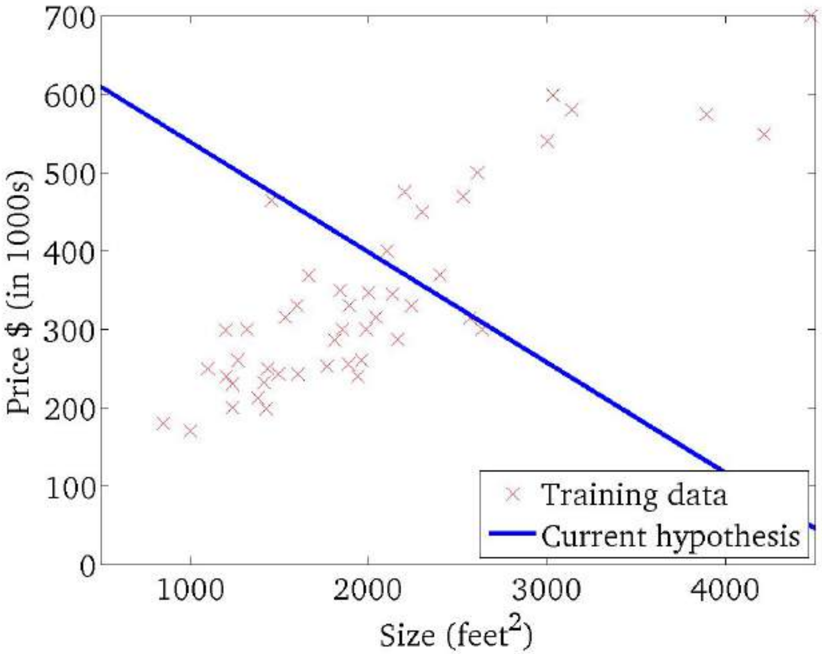
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



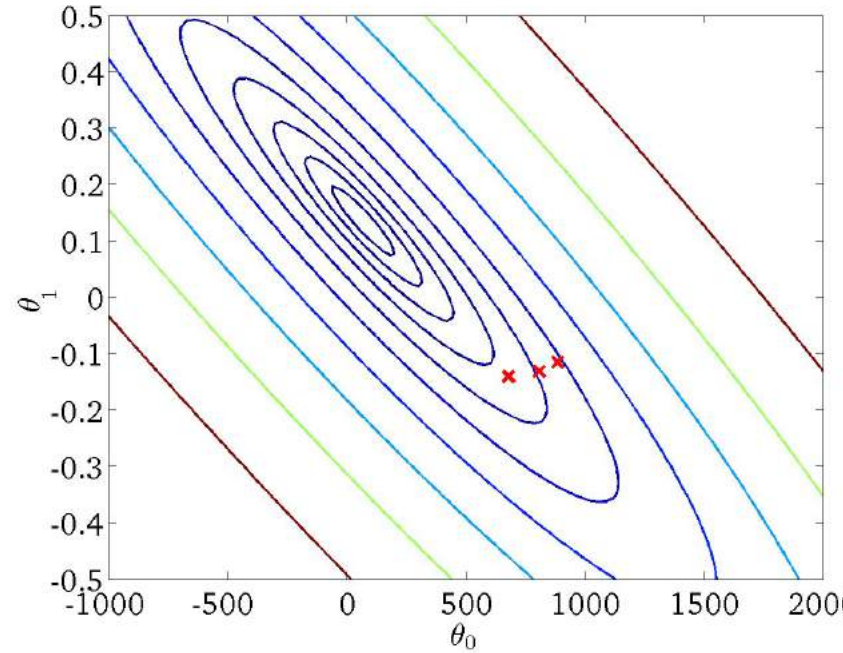
$h_\theta(x)$

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



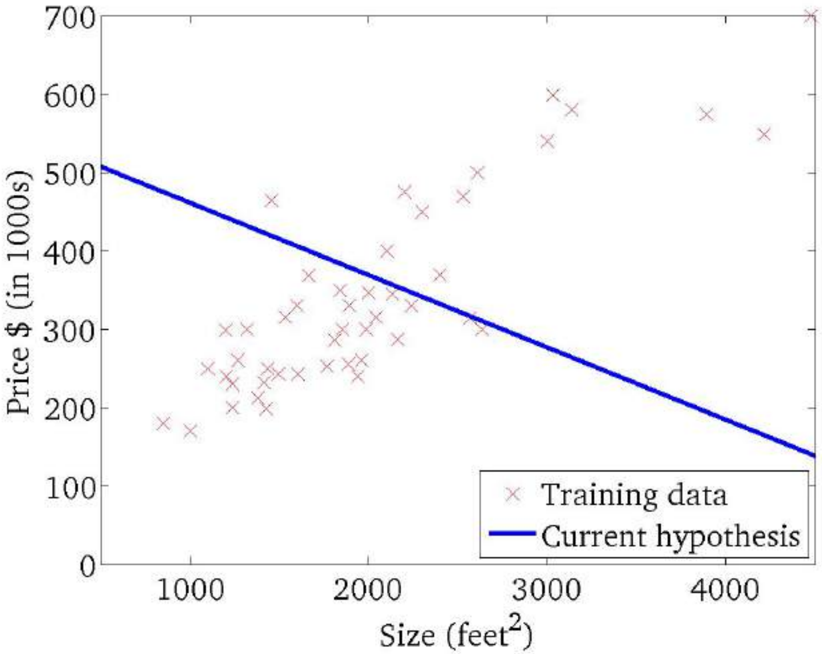
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



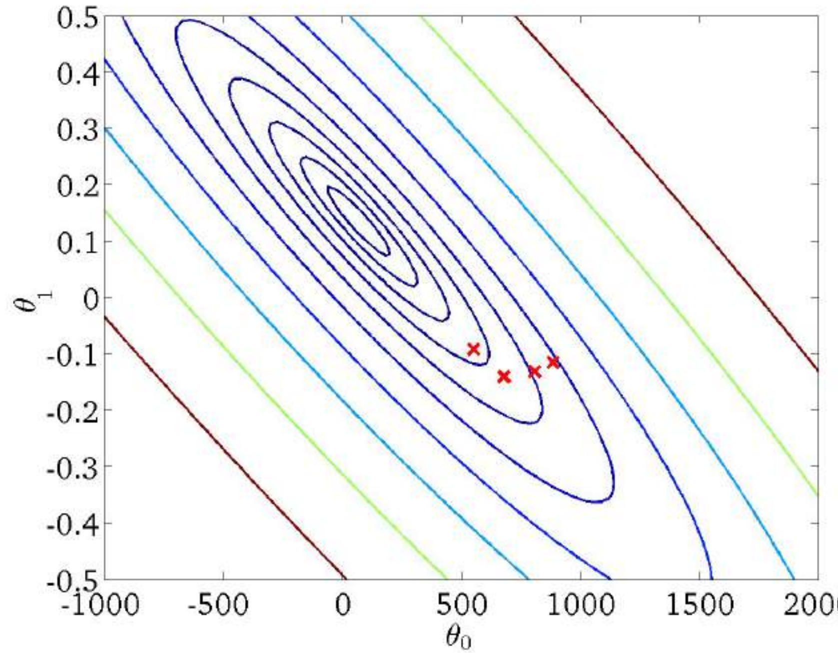
$h_\theta(x)$

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



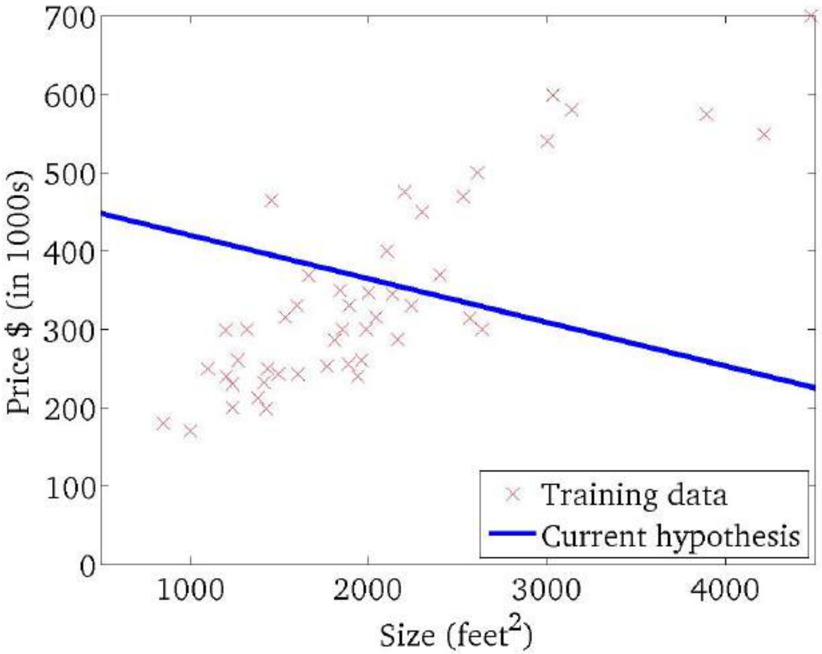
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



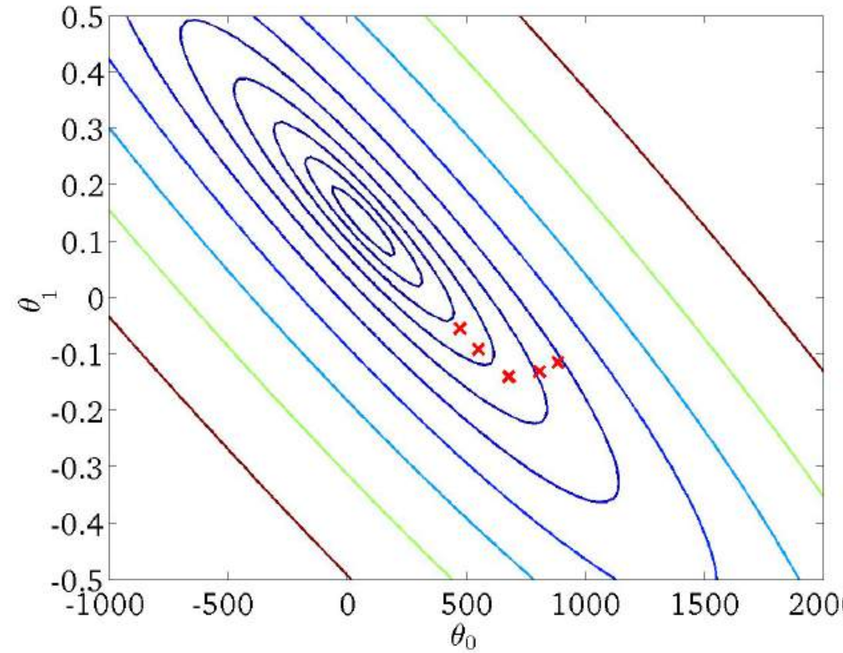
$h_\theta(x)$

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



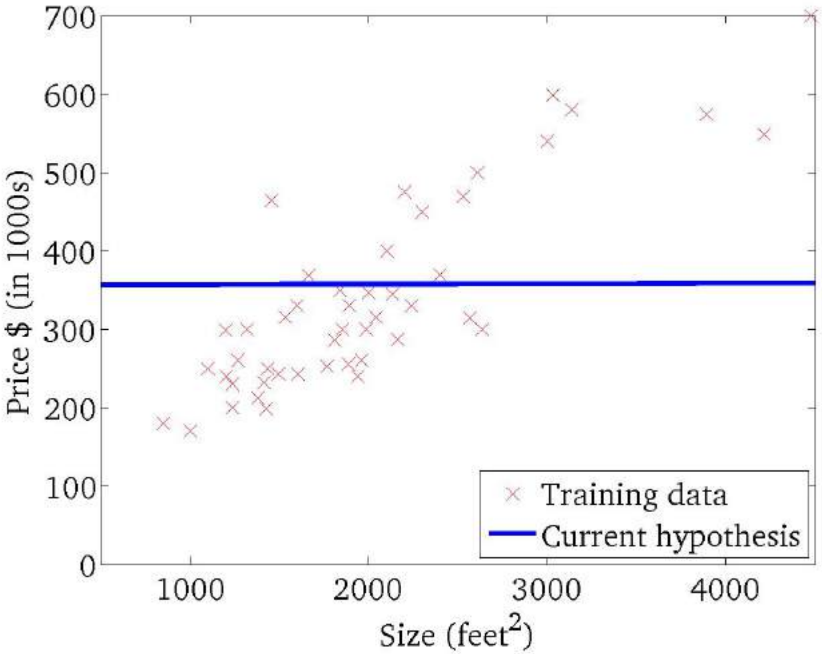
$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



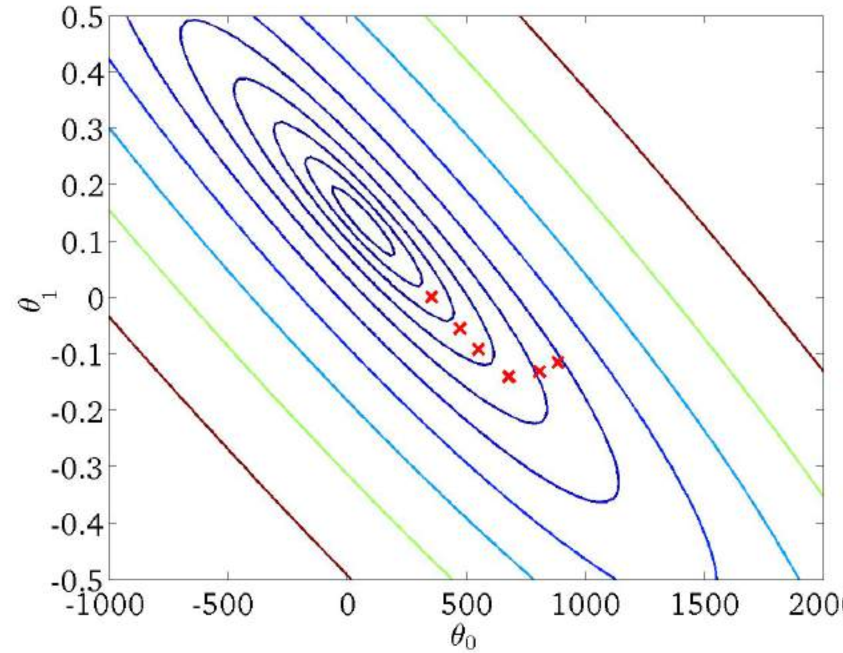
$$h_\theta(x)$$

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



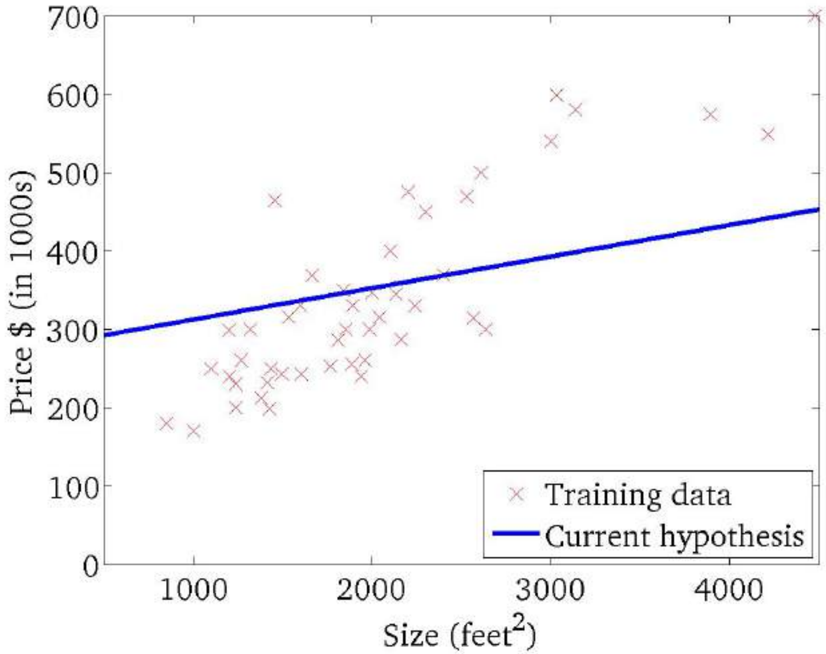
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



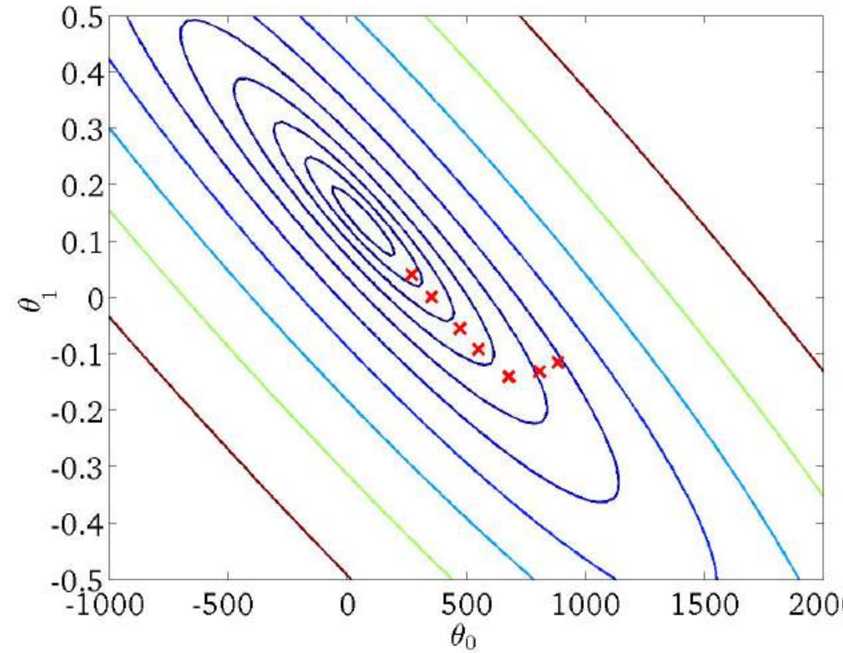
$$h_\theta(x)$$

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



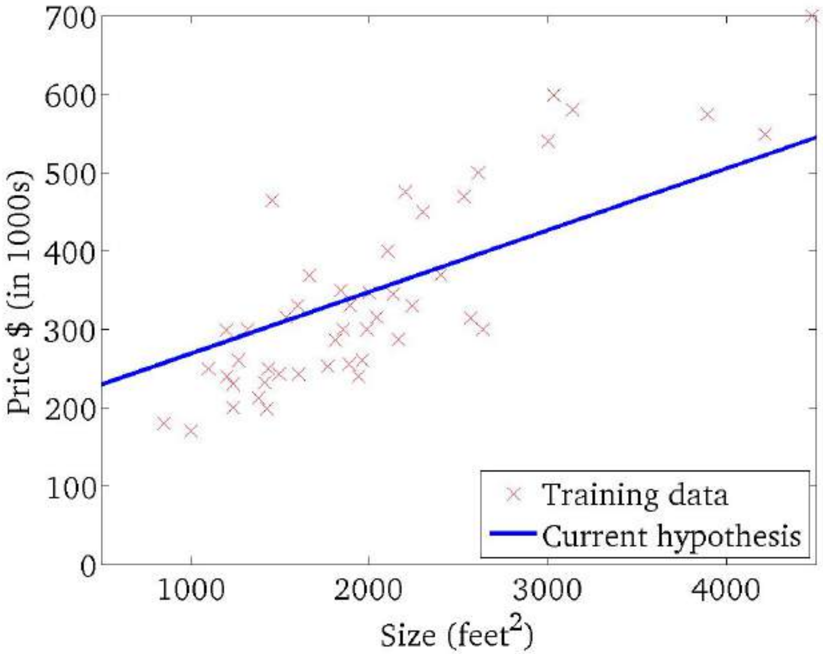
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



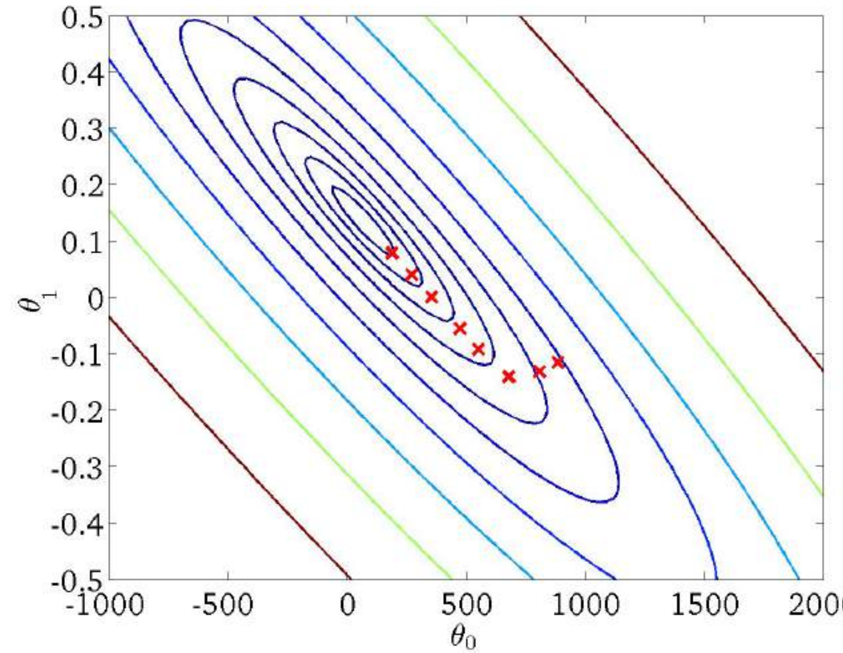
$$h_\theta(x)$$

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



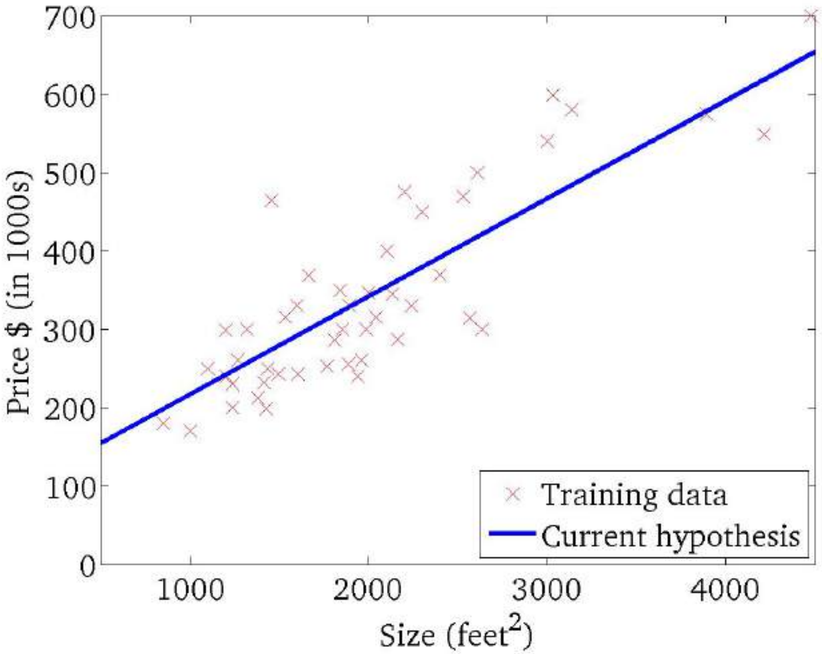
$$J(\theta_0, \theta_1)$$

(function of the parameters θ_0, θ_1)



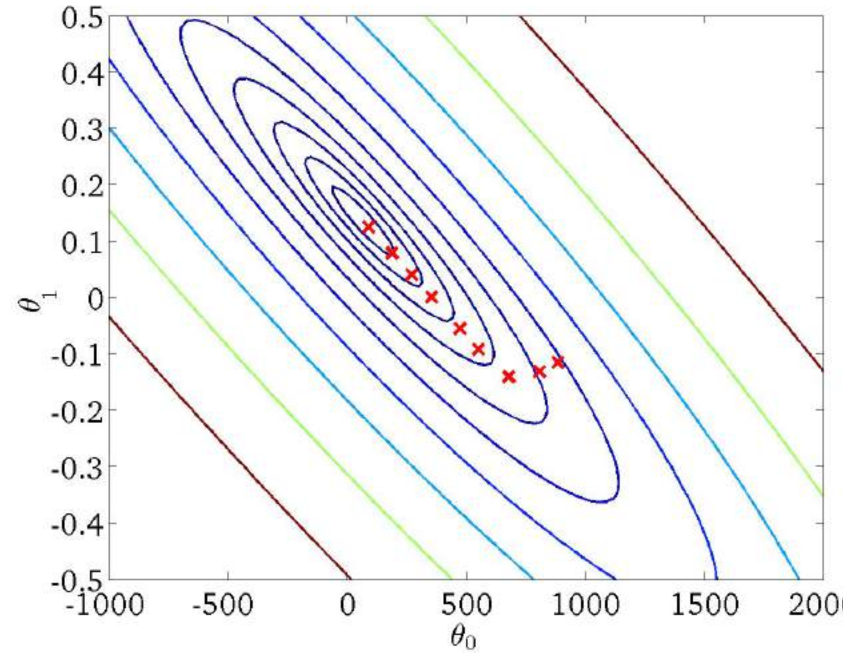
$$h_\theta(x)$$

(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.

https://stats.stackexchange.com/questions/49528/batch-gradient-descent-versus-stochastic-gradient-descent

Linear Regression with multiple variables

Multiple features

Multiple features (variables).

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

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

Multiple features (variables).

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

Notation:

n = number of features

$x^{(i)}$ = input (features) of i^{th} training example.

$x_j^{(i)}$ = value of feature j in i^{th} training example.

Hypothesis:

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

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

For convenience of notation, define $x_0 = 1$.

Multivariate linear regression.

Linear Regression with multiple variables

Gradient descent for multiple variables

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

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

Cost function:

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

Gradient descent:

Repeat $\{$

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

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

Gradient Descent

Previously (n=1):

Repeat $\{$

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

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

(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 $j = 0, \dots, n$)

$\}$

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

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

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

$\dots$

Linear Regression with multiple variables

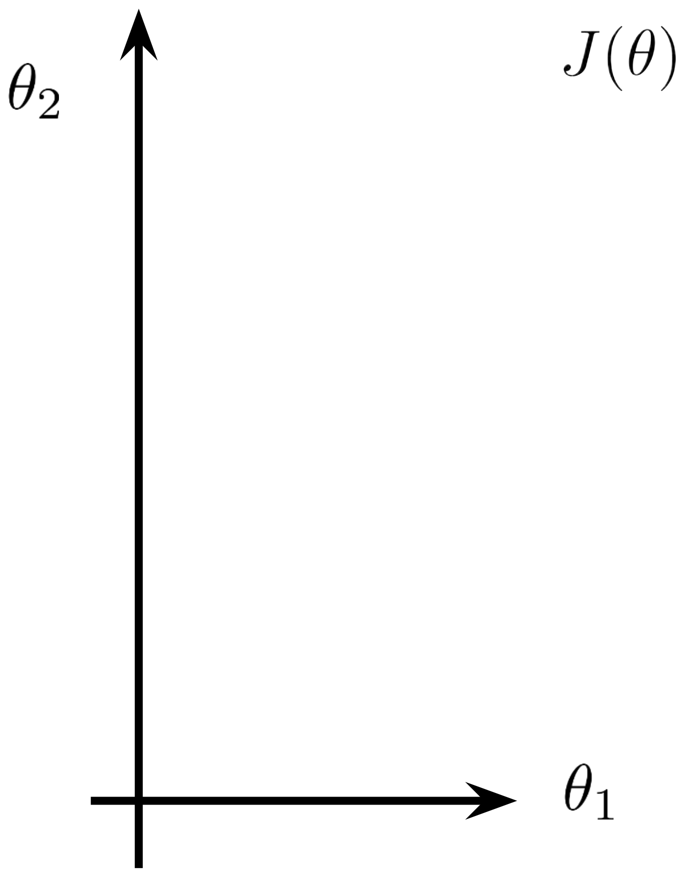
Gradient descent in practice I: Feature Scaling

Feature Scaling

Idea: Make sure features are on a similar scale.

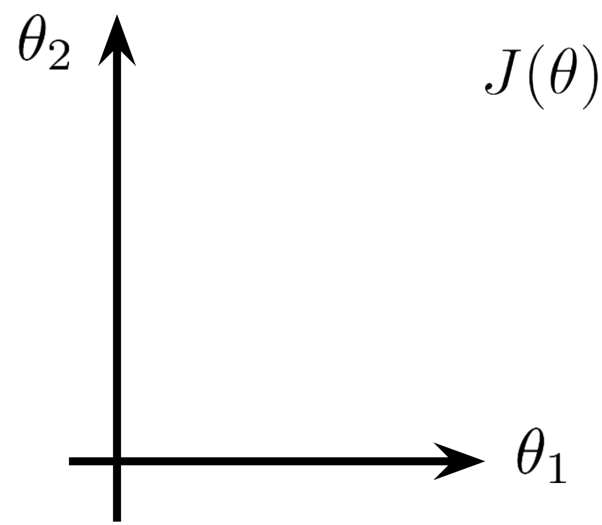
E.g. x_1 = size (0-2000 feet^2)

x_2 = number of bedrooms (1-5)



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

$$x_2 = \frac{numbersdfofbedrooms}{5}$$



Feature Scaling

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

Mean normalization

Replace x_i with $x_i - \mu_i$ to make features have approximately zero mean (Do not apply to $x_0 = 1$).

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

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

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

Linear Regression with multiple variables

Gradient descent in practice II: Learning rate

Gradient descent

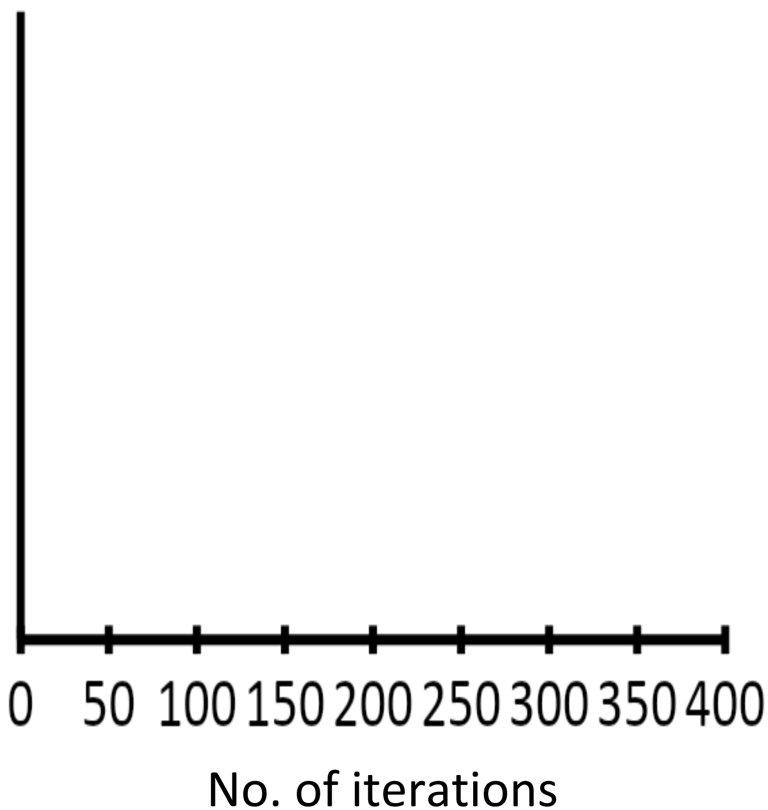
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

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

- How to choose learning rate α.

Making sure gradient descent is working correctly.

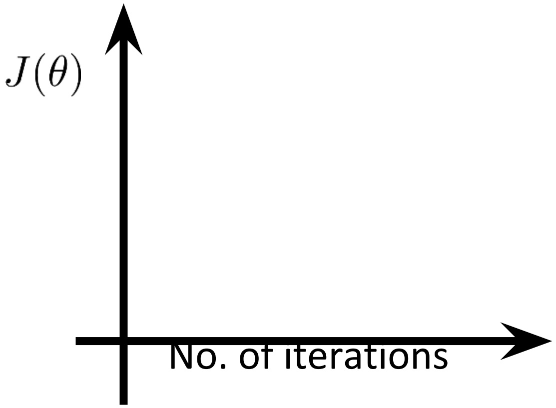
$$\min_{\theta} J(\theta)$$



Example automatic convergence test:

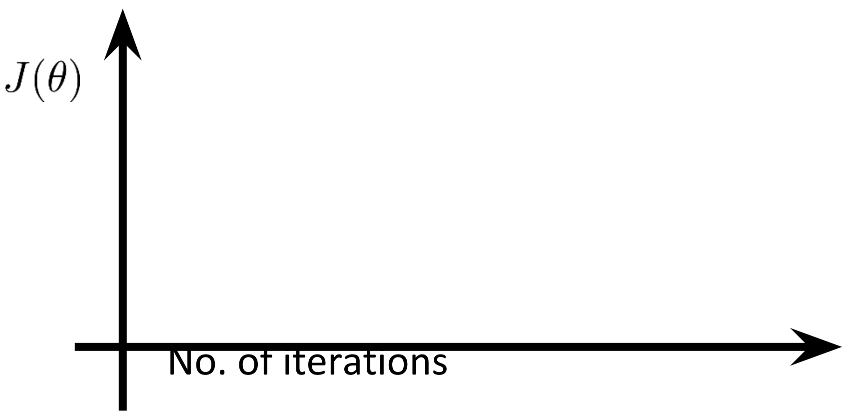
Declare convergence if $J(\theta)$ decreases by less than 10^{-3} in one iteration.

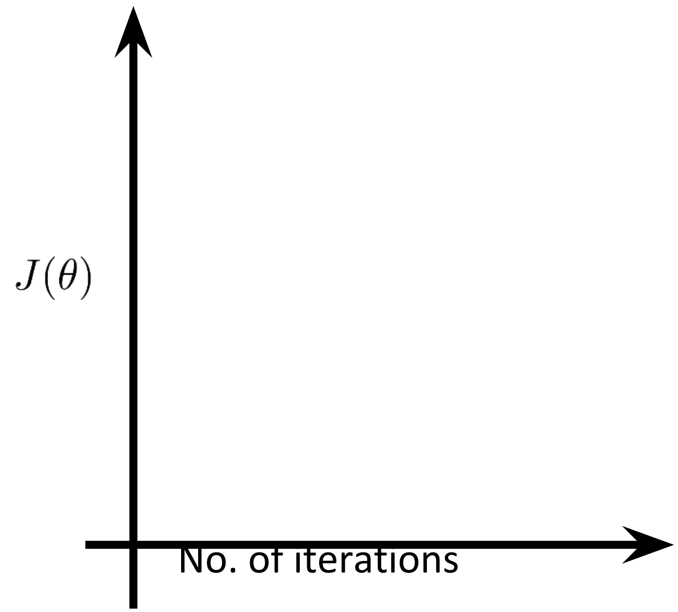
Making sure gradient descent is working correctly.



Gradient descent not working.

Use smaller α.





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

Summary:

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

To choose α, try

$$\ldots, 0.001, \qquad , 0.01, \qquad , 0.1, \qquad , 1, \ldots$$

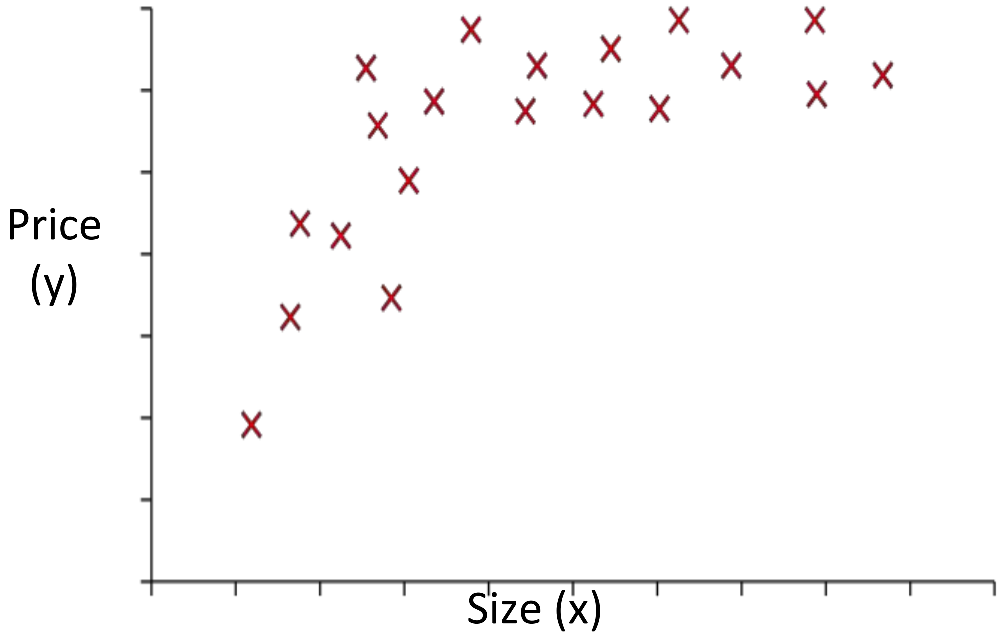
Linear Regression with multiple variables

Features and polynomial regression

Housing prices prediction

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

Polynomial regression



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

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

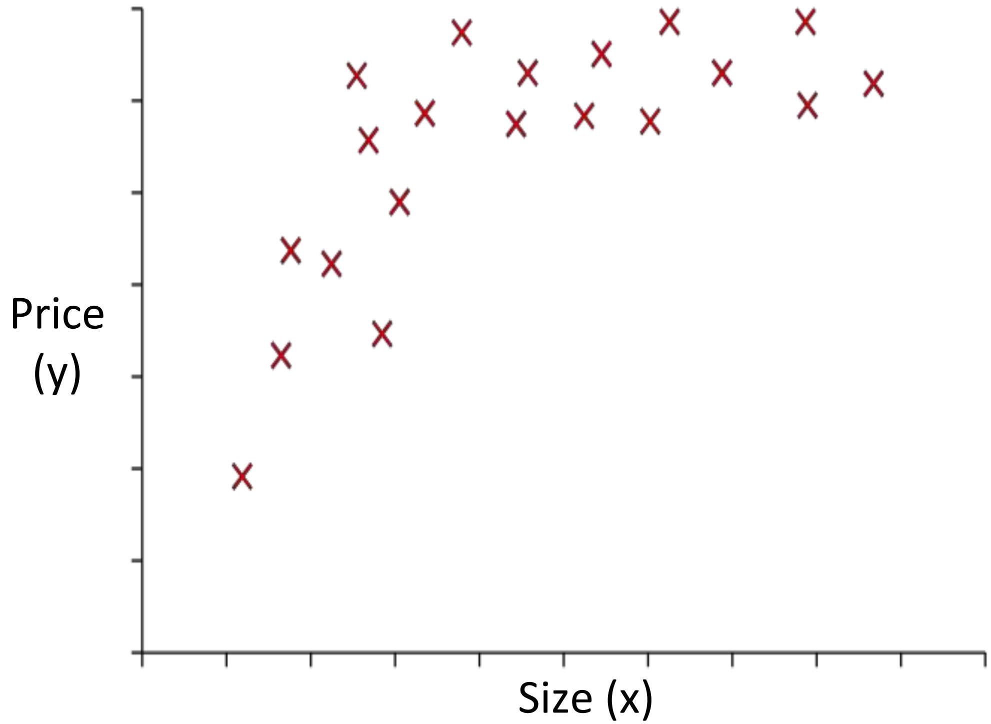
$$\begin{aligned} h_\theta(x) &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 \\ &= \theta_0 + \theta_1 (size) + \theta_2 (size)^2 + \theta_3 (size)^3 \end{aligned}$$

$$x_1 = (size)$$

$$x_2 = (size)^2$$

$$x_3 = (size)^3$$

Choice of features



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

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

Logistic Regression

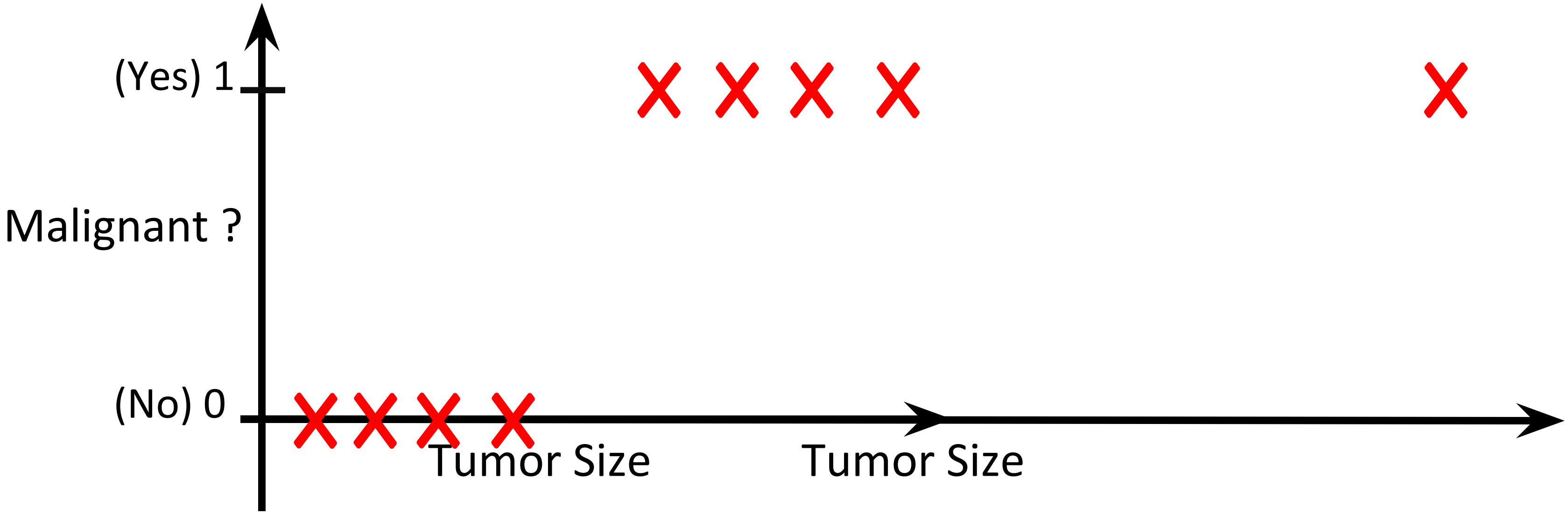
Classification

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)



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

Logistic Regression

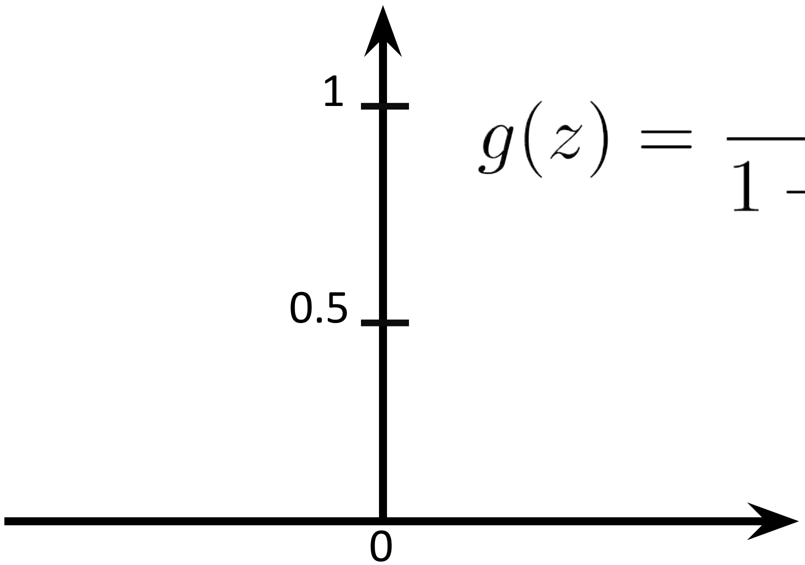
Hypothesis Representation

Logistic Regression Model

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

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

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



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

Sigmoid function
Logistic function

Interpretation of Hypothesis Output

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

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

$$h_\theta(x) = 0.7$$

Tell patient that 70% chance of tumor being malignant

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

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

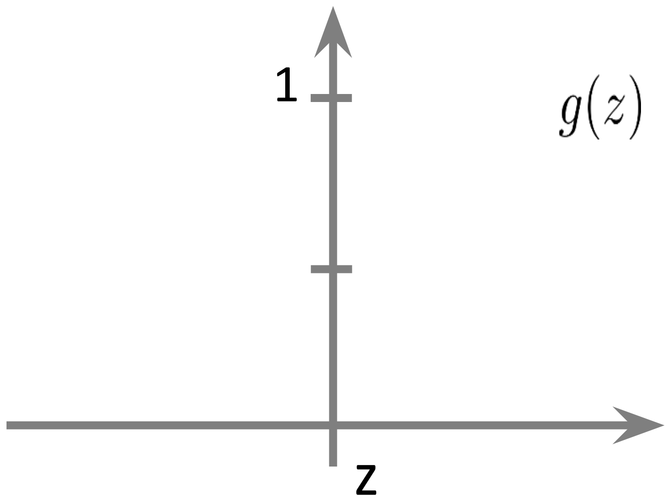
Logistic Regression

Decision boundary

Logistic regression

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

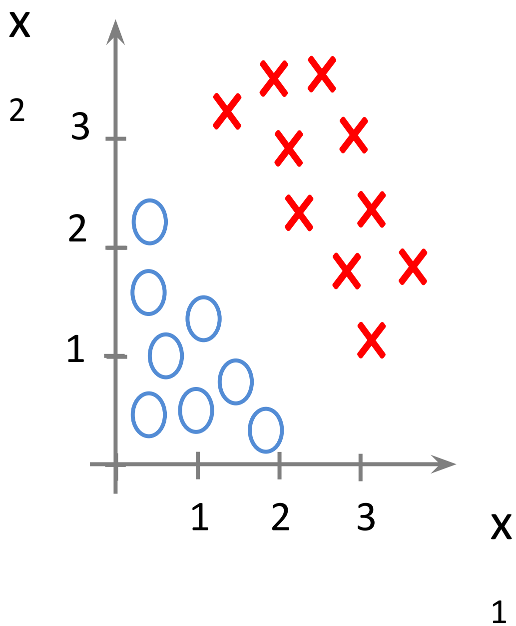
$$g(z) = \frac{1}{1+e^{-z}}$$



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

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

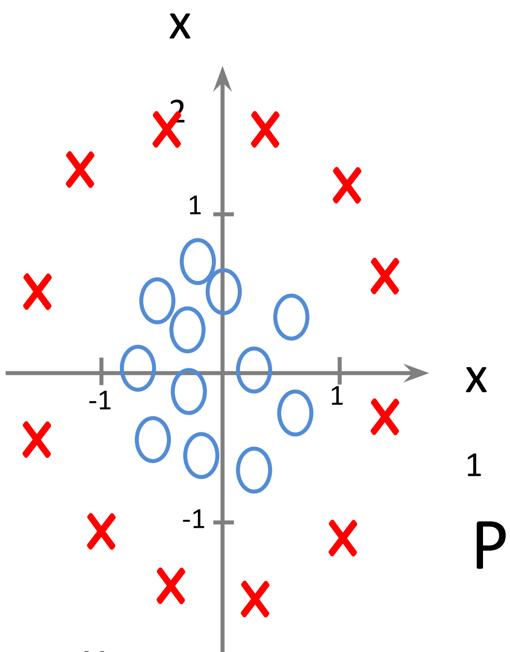
Decision Boundary



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

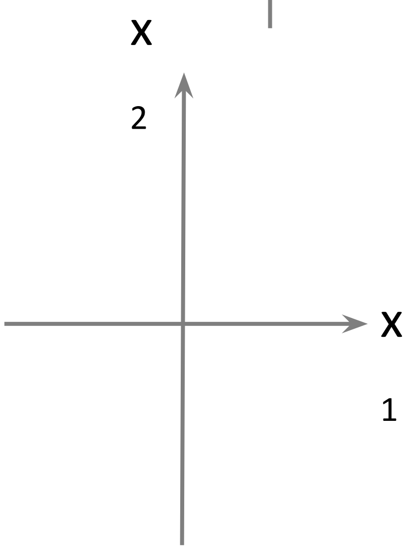
Predict "$y = 1$" if $-3 + x_1 + x_2 \geq 0$

Non-linear decision boundaries



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

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



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

Logistic Regression

Cost function

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

m examples

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

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

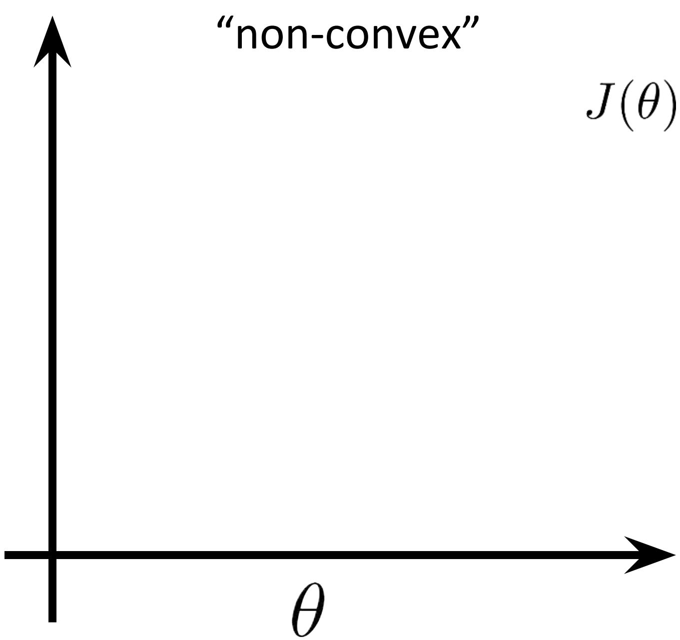
How to choose parameters θ ?

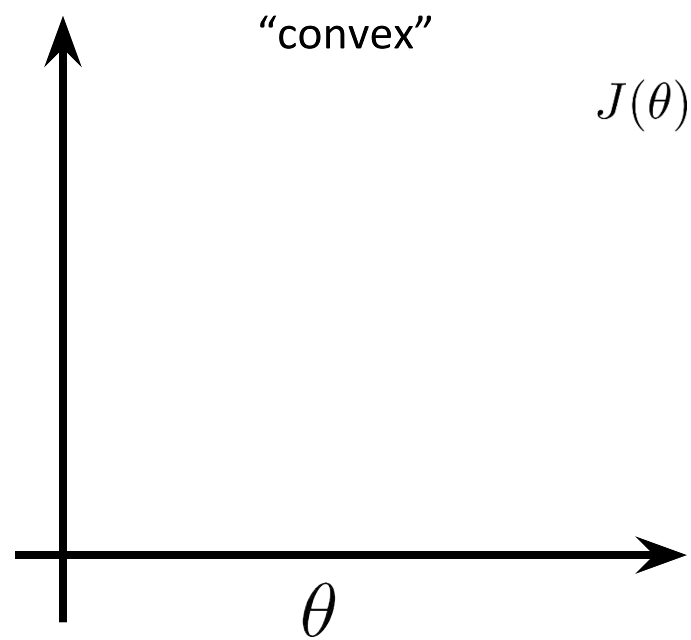
Cost function

https://stats.stackexchange.com/questions/324561/difference-between-convex-and-concave-functions

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

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

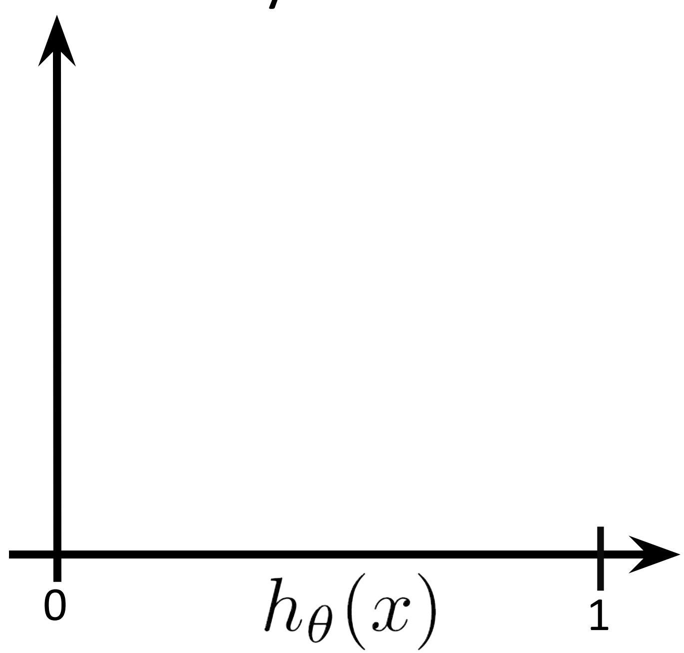




Logistic regression cost function

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

If y = 1



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

Simplified cost function and gradient descent

Logistic regression cost function

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

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

Note: $y = 0$ or 1 always

To fit parameters θ :

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

To make a prediction given new x:

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

Gradient Descent

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)

$\}$

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:

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}$$

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

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

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

```
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 = $\begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$

```
function [jVal, gradient] = costFunction(theta)

    jVal = [code to compute J(θ)];

    gradient(1) = [code to compute ∂/∂θ_0 J(θ)];

    gradient(2) = [code to compute ∂/∂θ_1 J(θ)];

     ⋮

    gradient(n+1) = [code to compute ∂/∂θ_n J(θ)];
```

$$\texttt{jVal = [}\text{code to compute } J(\theta)\texttt{];}$$

$$\texttt{gradient(1) = [}\text{code to compute } \frac{\partial}{\partial\theta_0}J(\theta)\texttt{];}$$

$$\texttt{gradient(2) = [}\text{code to compute } \frac{\partial}{\partial\theta_1}J(\theta)\texttt{];}$$

$$\vdots$$

$$\texttt{gradient(n+1) = [}\text{code to compute } \frac{\partial}{\partial\theta_n}J(\theta)\texttt{];}$$

Logistic Regression

Multi-class classification:
One-vs-all

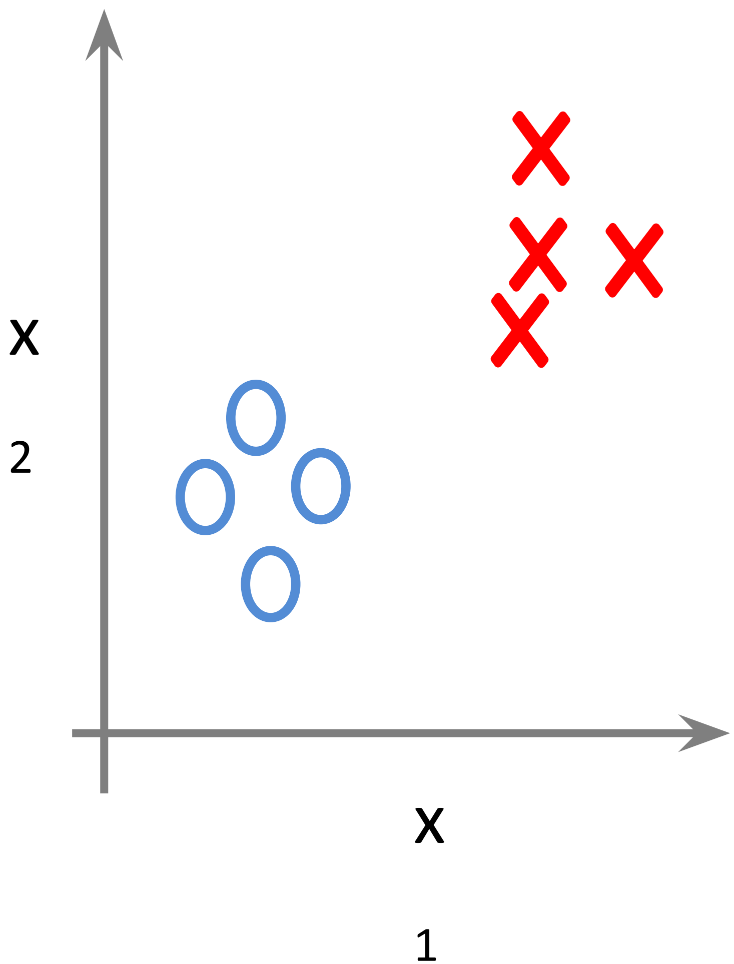
Multiclass classification

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

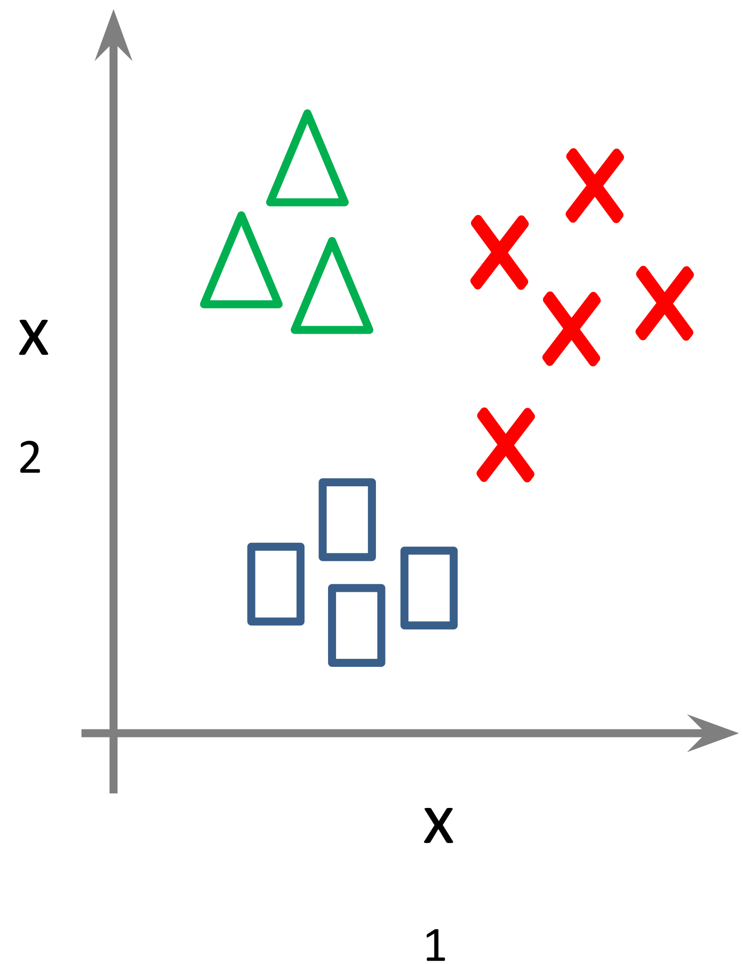
Medical diagrams: Not ill, Cold, Flu

Weather: Sunny, Cloudy, Rain, Snow

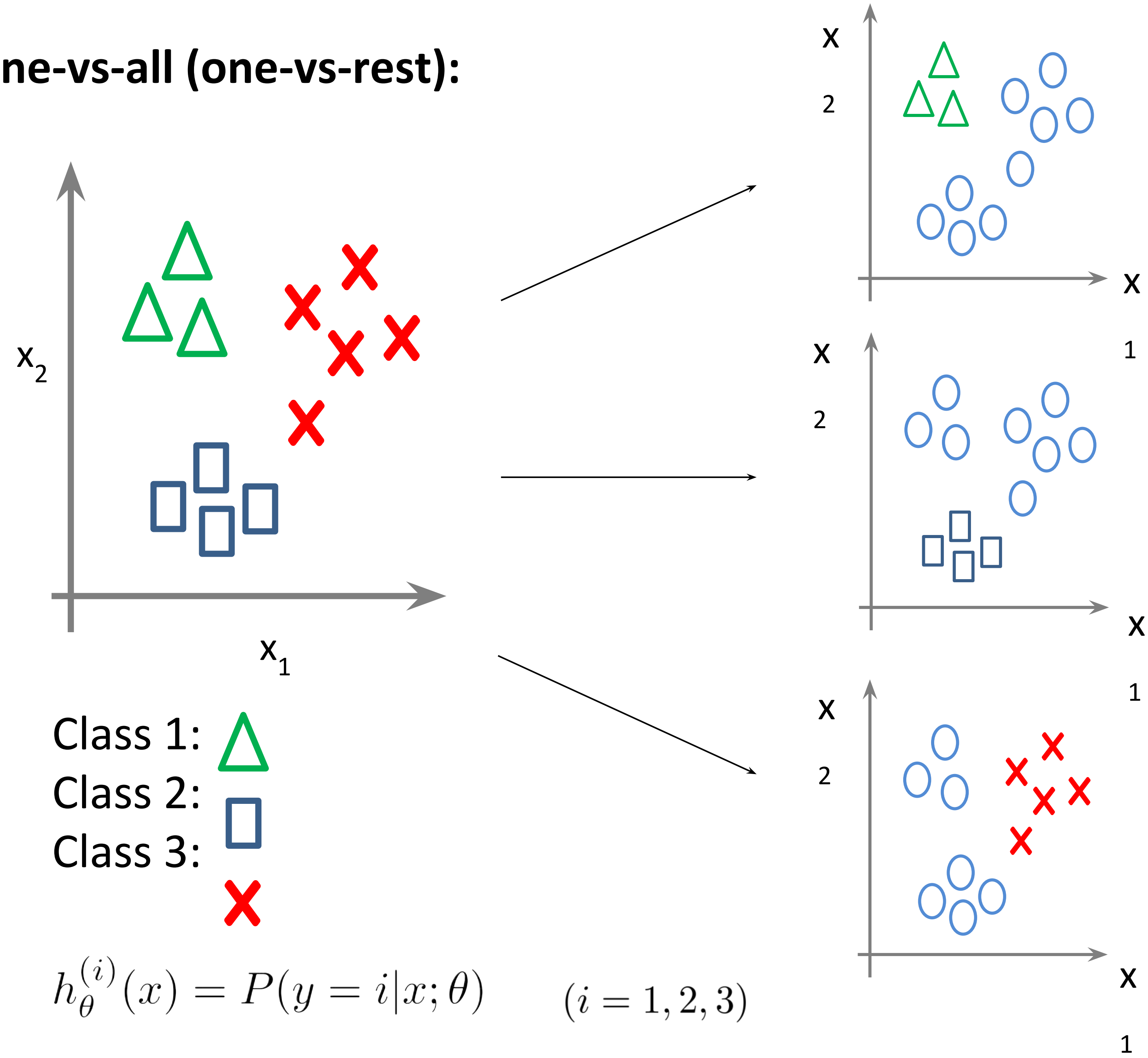
Binary classification:



Multi-class classification:



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



Class 1:
Class 2:
Class 3:

$$h_\theta^{(i)}(x) = P(y = i|x;\theta) \qquad (i = 1, 2, 3)$$

One-vs-all

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

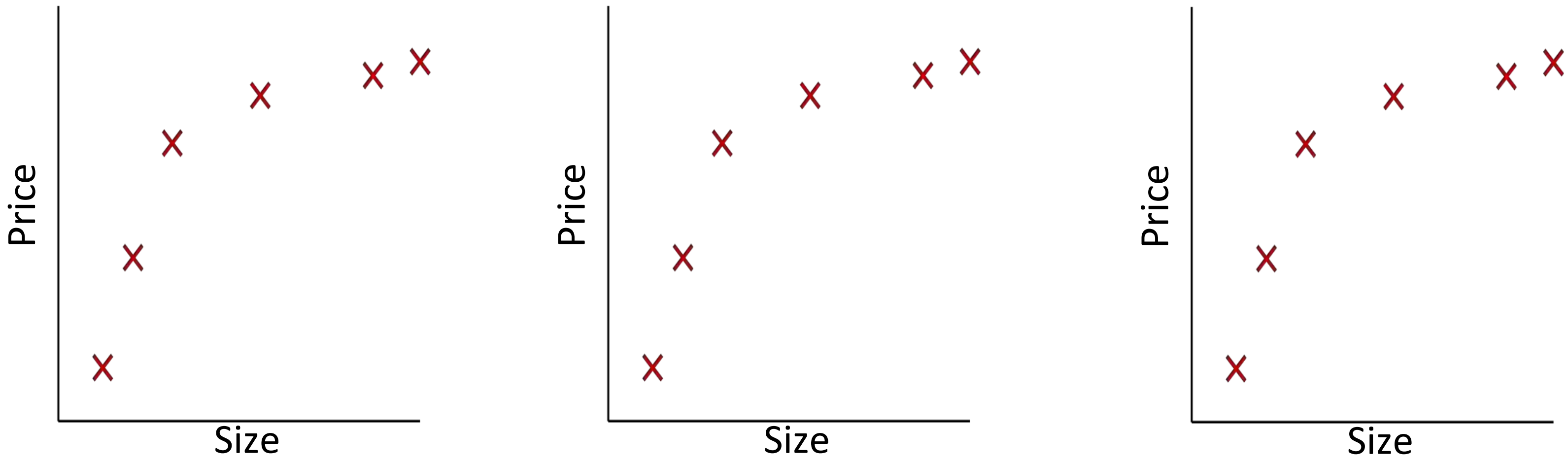
On a new input x, to make a prediction, pick the class i that maximizes

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

Regularization

The problem of overfitting

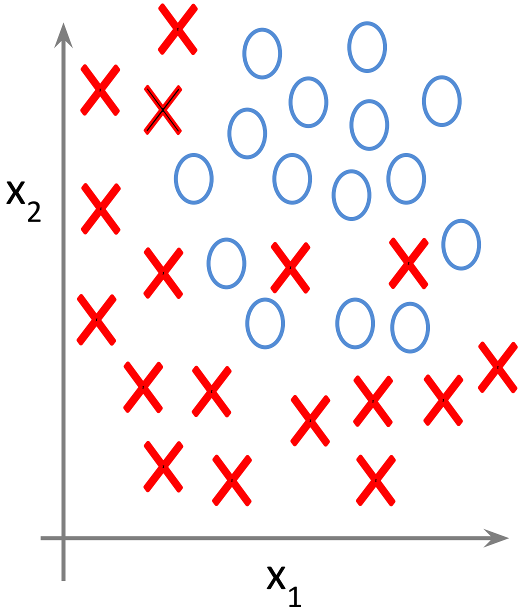
Example: Linear regression (housing prices)

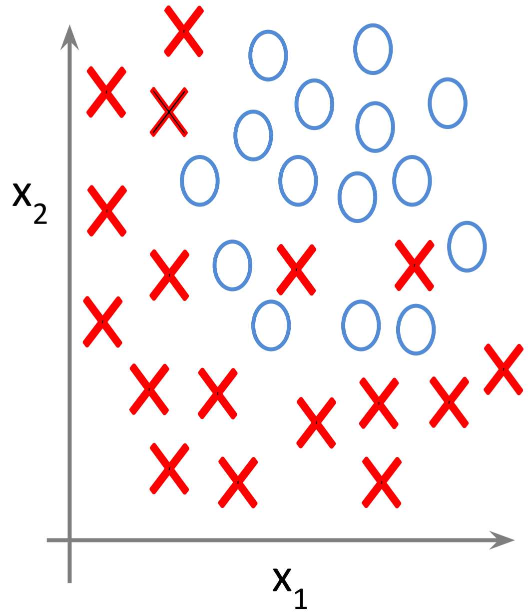


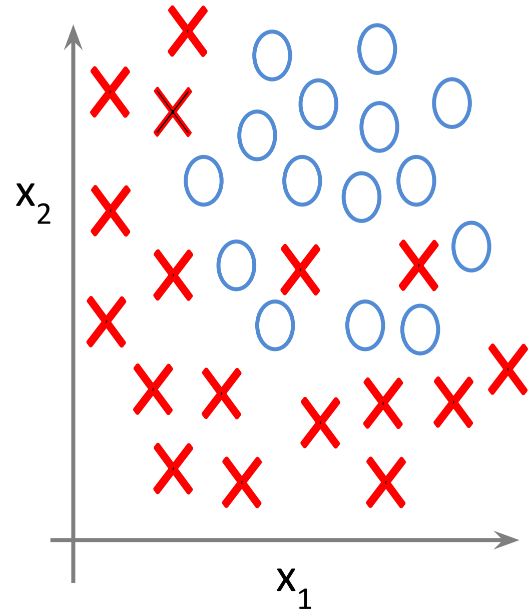
$\theta_0 + \theta_1 x$ $\quad$ $\theta_0 + \theta_1 x + \theta_2 x^2$ $\quad$ $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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)

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

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

Addressing overfitting:

$x_1 =$ size of house

$x_2 =$ no. of bedrooms

$x_3 =$ no. of floors

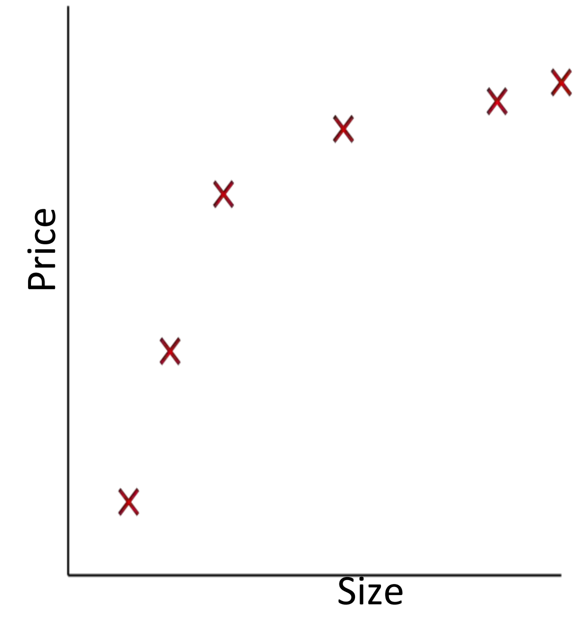
$x_4 =$ age of house

$x_5 =$ average income in neighborhood

$x_6 =$ kitchen size

$\vdots$

x_{100}



Addressing overfitting:

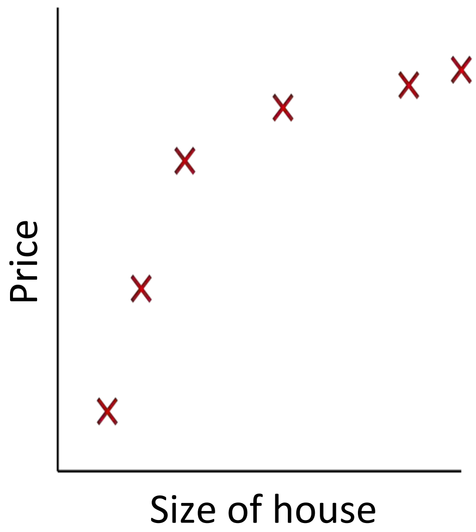
Options:

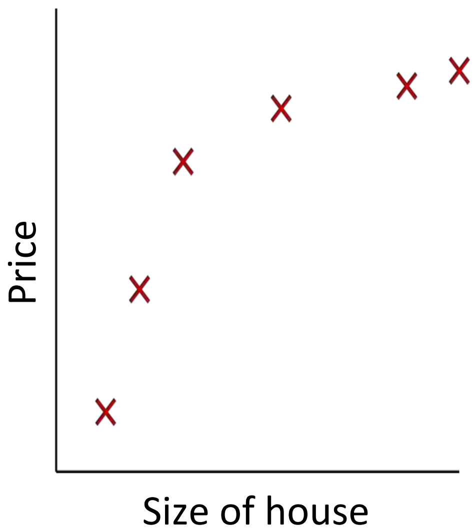
1. Reduce number of features.
   - Manually select which features to keep.
   - Model selection algorithm (later in course).
2. Regularization.
   - Keep all the features, but reduce magnitude/values of parameters θ_j.
   - Works well when we have a lot of features, each of which contributes a bit to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

Regularization

Cost function

Intuition





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

Suppose we penalize and make θ_3, θ_4 really small.

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

Regularization.

Small values for parameters $\theta_0, \theta_1, \ldots, \theta_n$
- "Simpler" hypothesis
- Less prone to overfitting

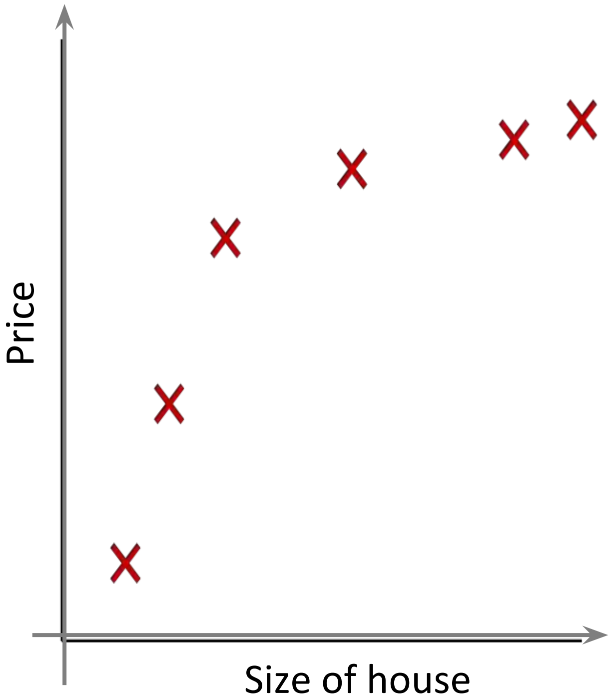
Housing:
- Features: $x_1, x_2, \ldots, x_{100}$
- Parameters: $\theta_0, \theta_1, \theta_2, \ldots, \theta_{100}$

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

Regularization.

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

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



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

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

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 $\{$

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

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

$$(j = \cancel{0}, 1, 2, 3, \ldots, n)$$

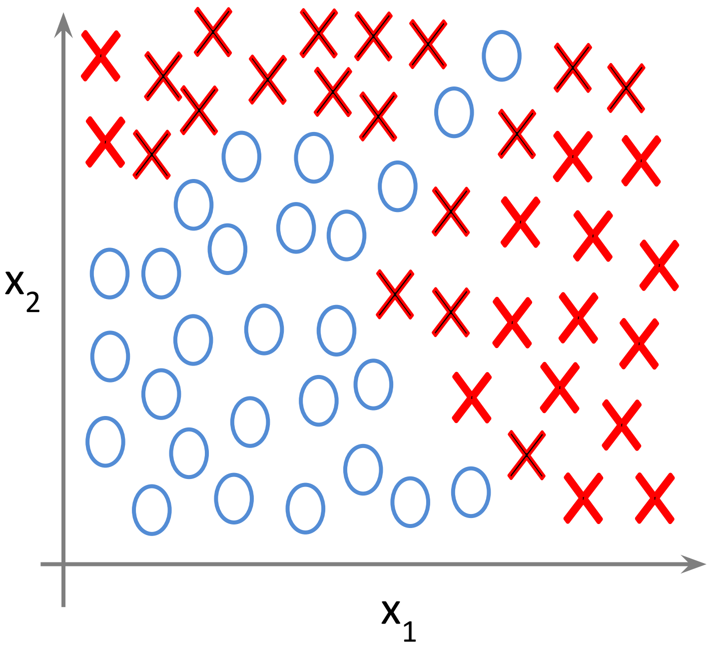
$\}$

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

Neural Networks: Representation

Non-linear hypotheses

Non-linear Classification



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

$x_1 =$ size

$x_2 =$ # bedrooms

$x_3 =$ # floors

$x_4 =$ age

$\ldots$

x_{100}

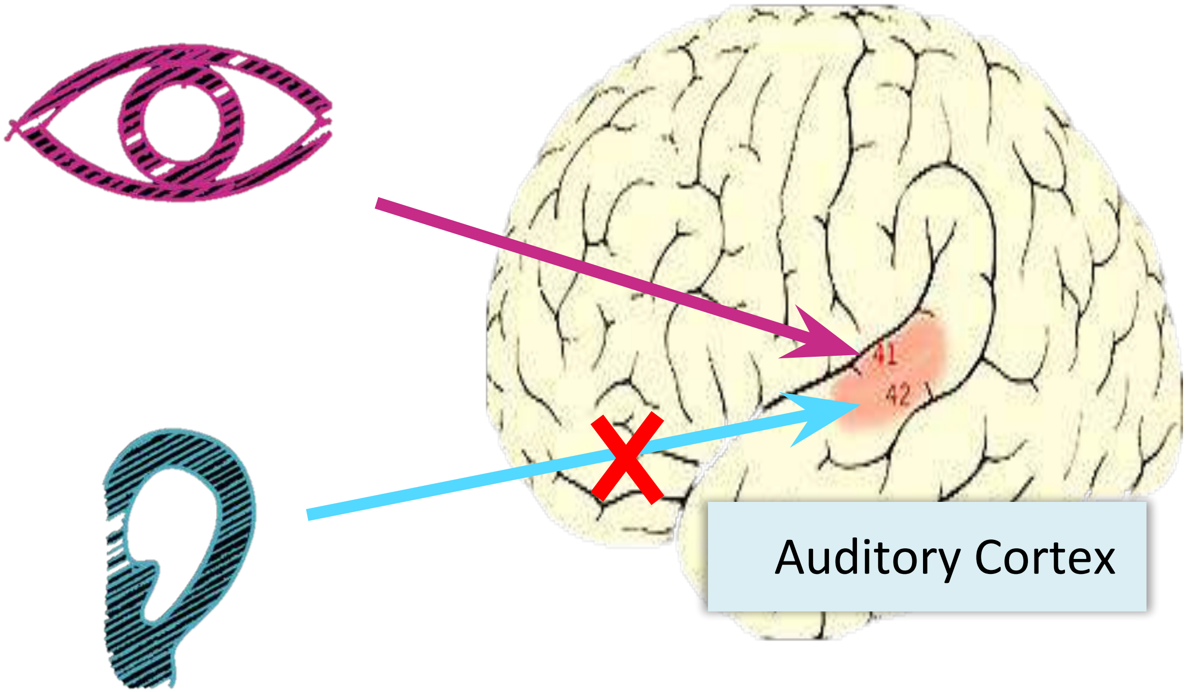
Neural Networks: Representation

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

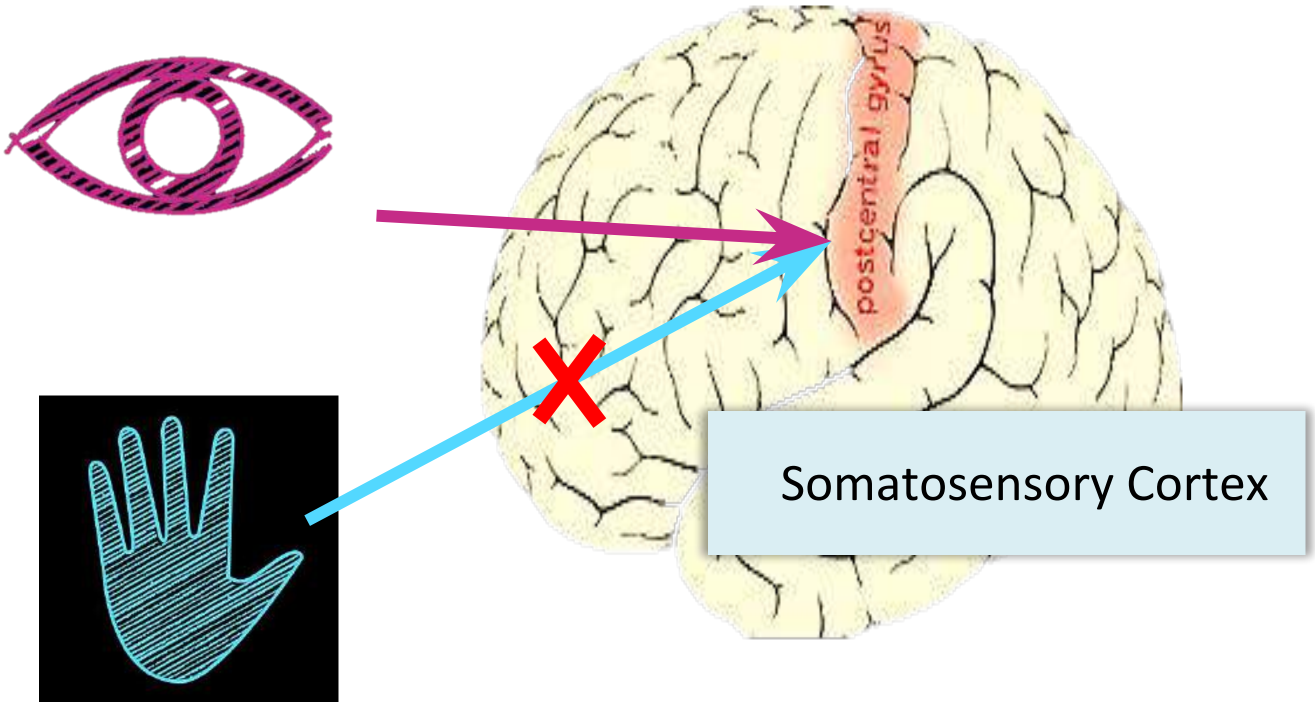
The “one learning algorithm” hypothesis



Auditory cortex learns to see

[Roe et al., 1992]

The “one learning algorithm” hypothesis



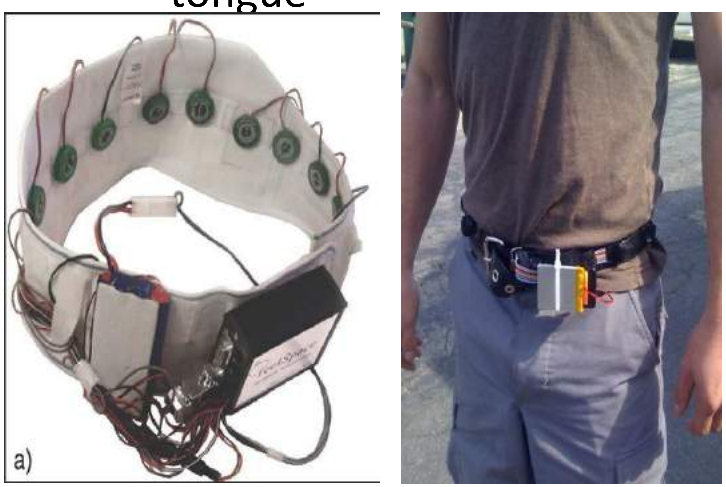
Somatosensory cortex learns to see

[Metin & Frost, 1989]

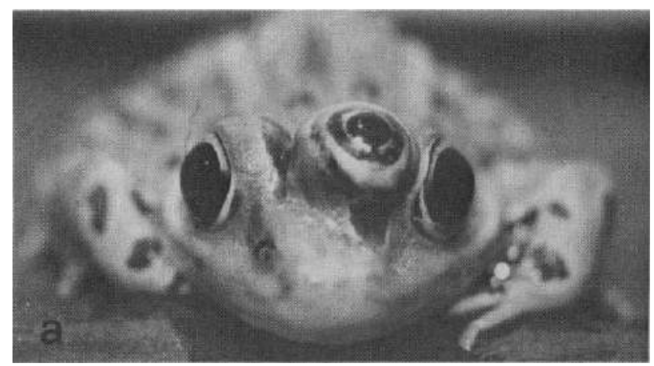
Sensor representations in the brain

Seeing with your tongue

Human echolocation (sonar)



Haptic belt: Direction sense



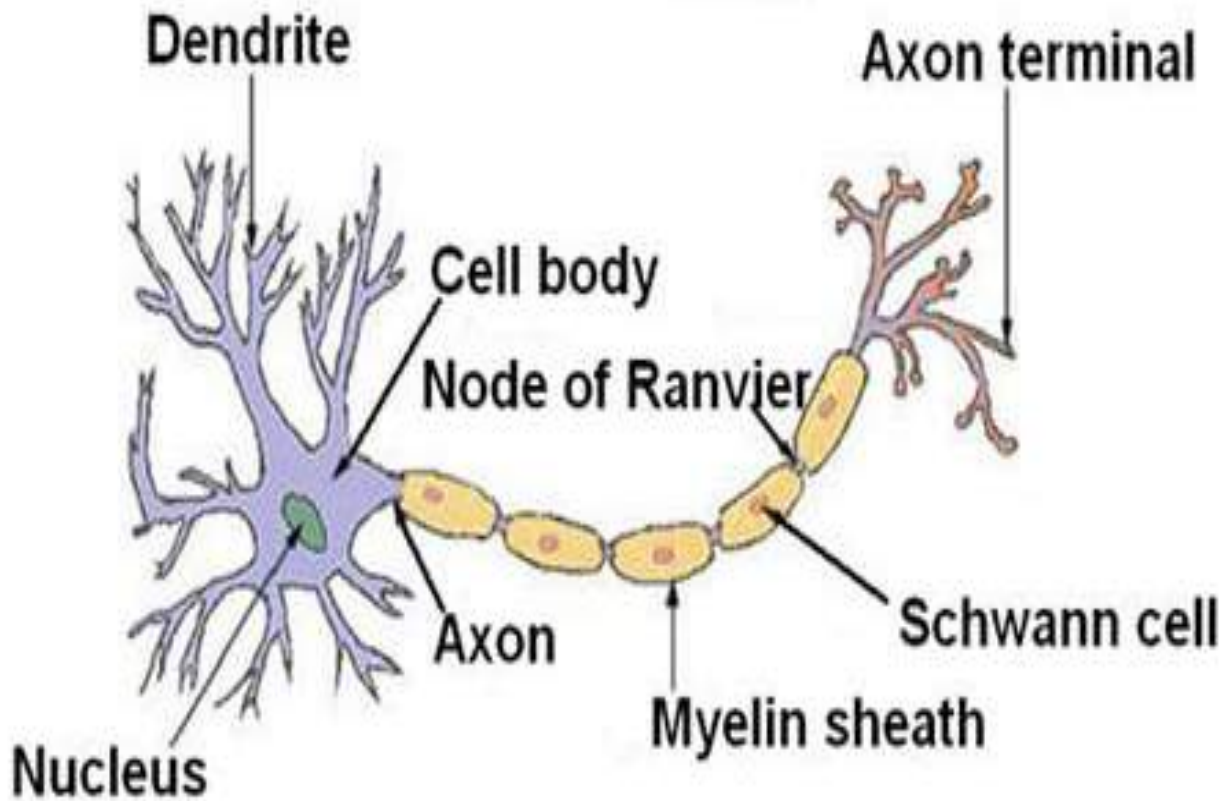
Implanting a 3rd eye

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

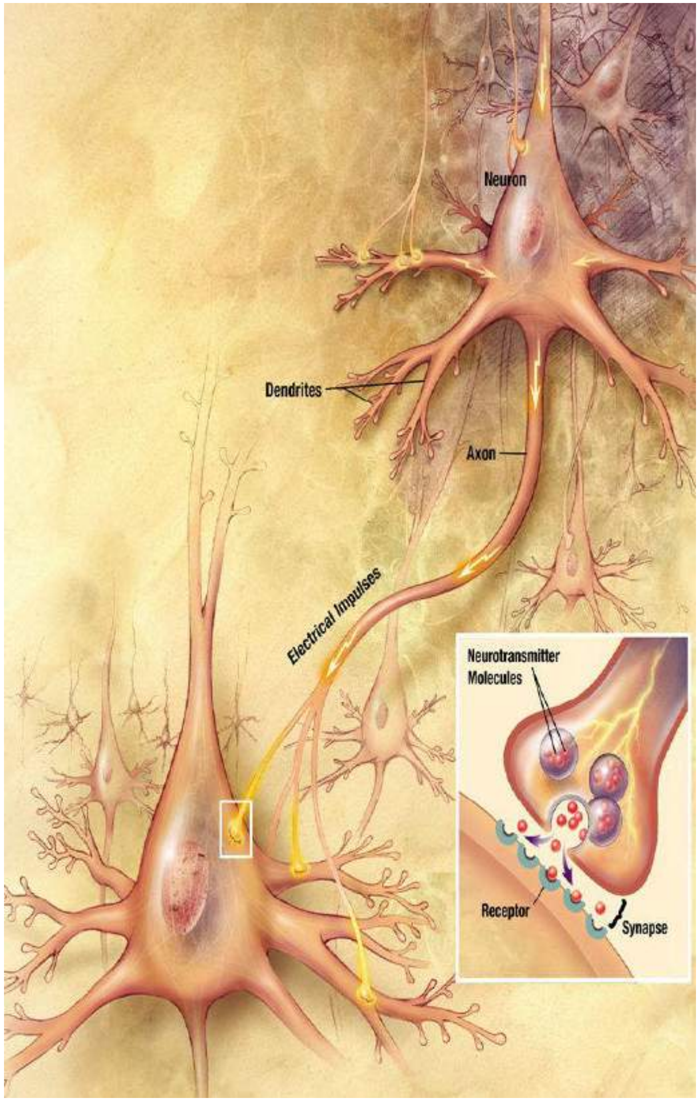
Neural Networks: Representation

Model representation I

Neuron in the brain



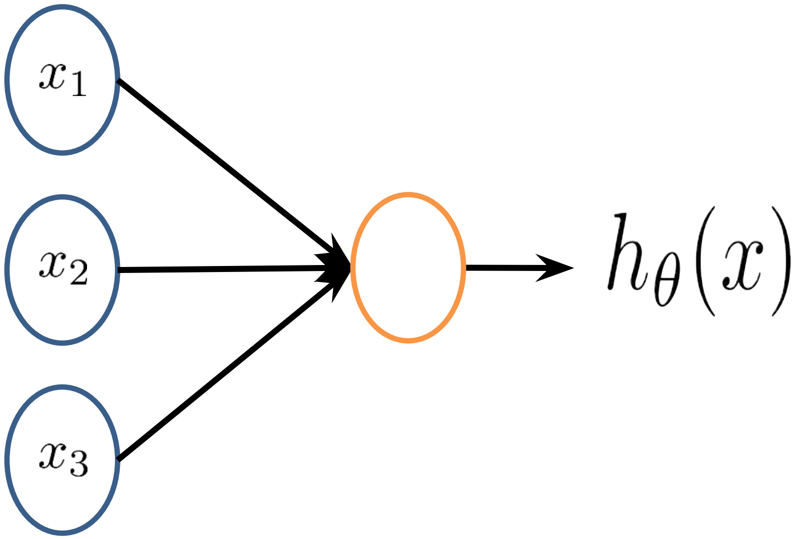
Neurons in the brain



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

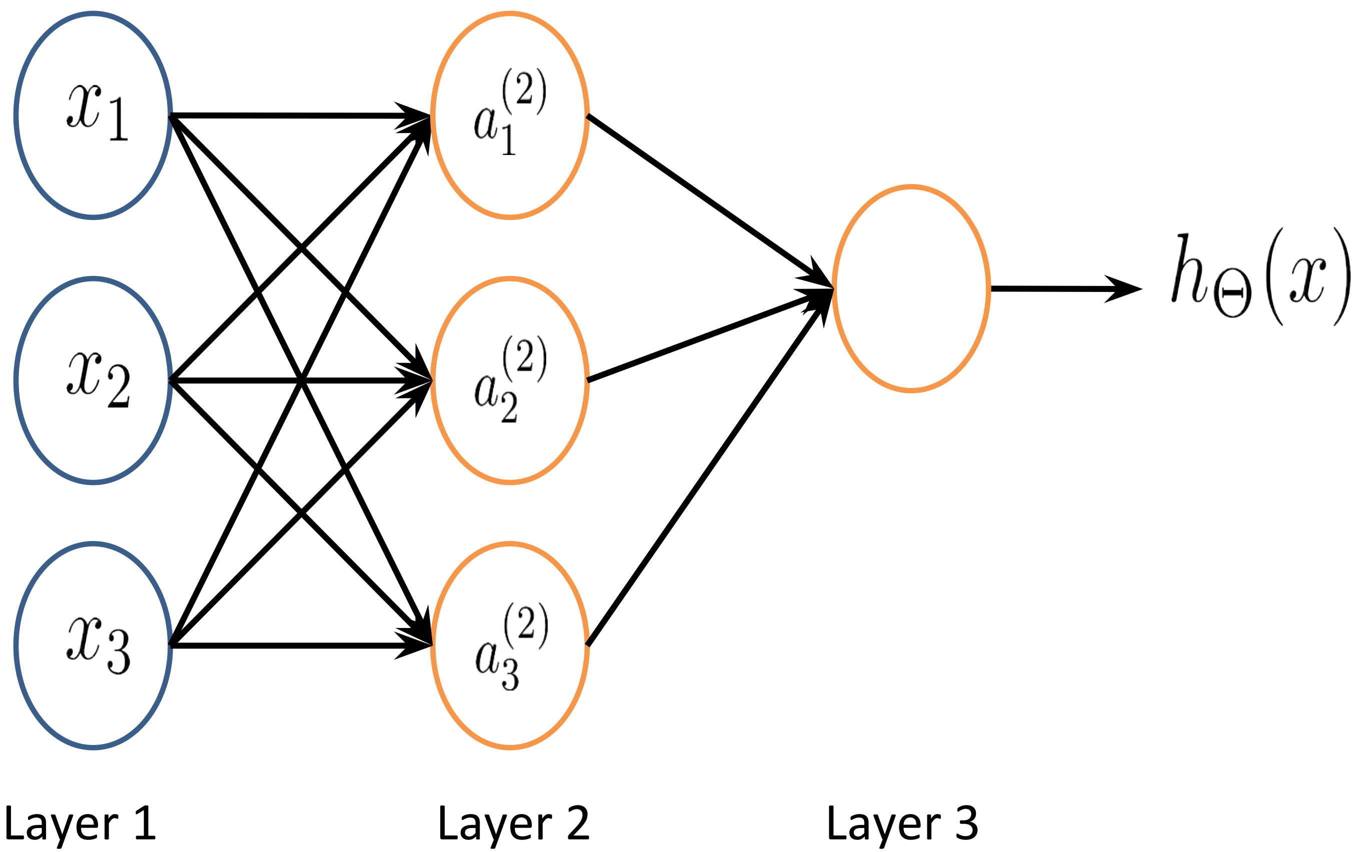
Neuron model: Logistic unit

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

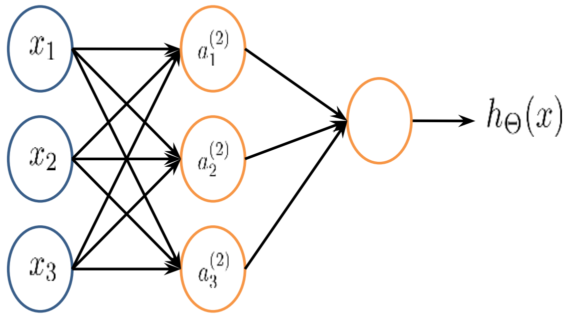


Sigmoid (logistic) activation function.

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 $j+1$

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

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

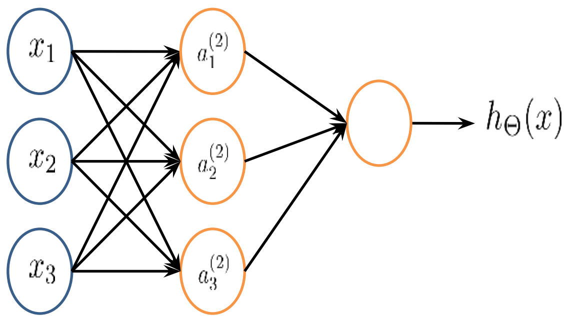
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$

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

Neural Networks: Representation

Model representation II

Forward propagation: Vectorized implementation



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

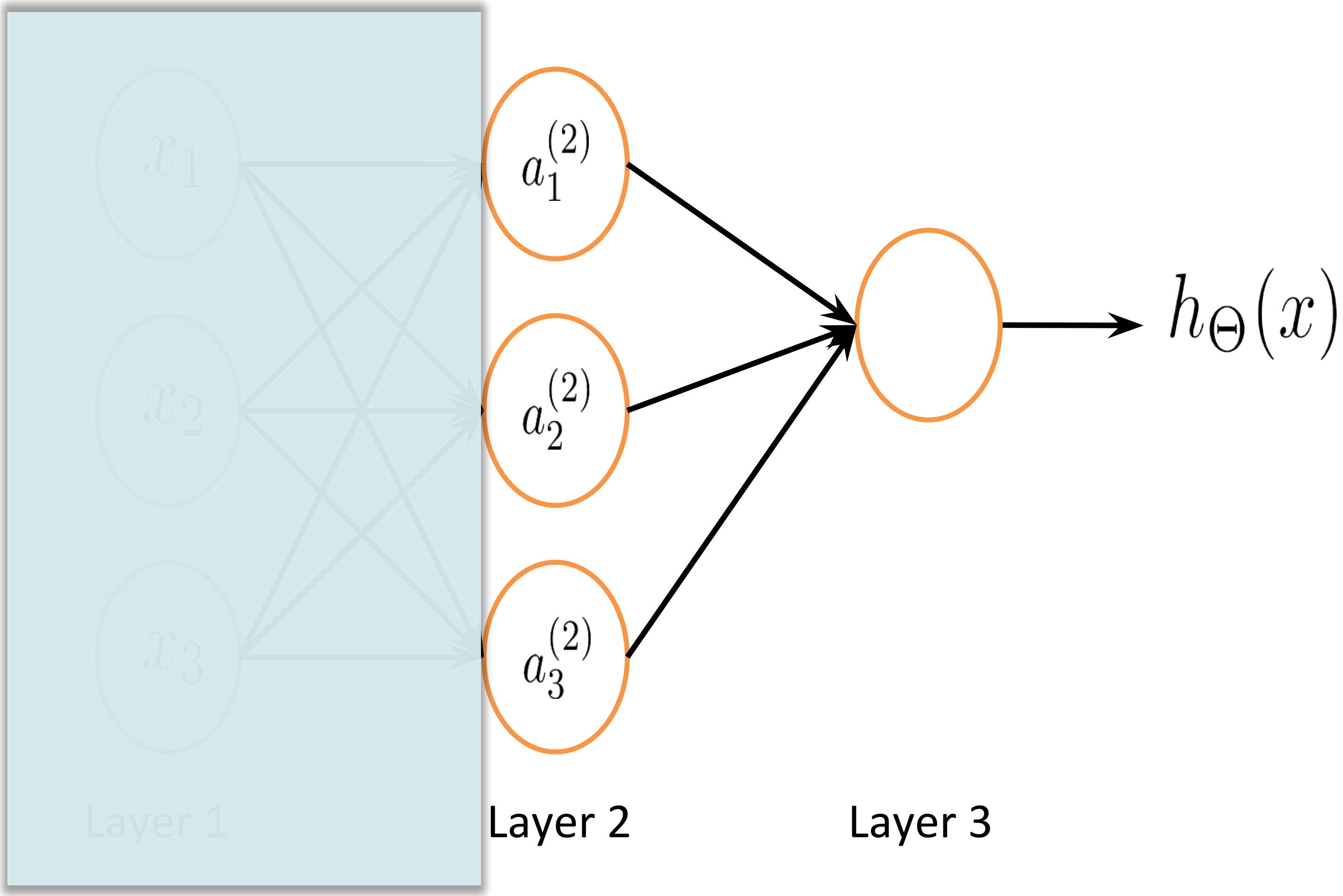
$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad z^{(2)} = \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix}$$

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

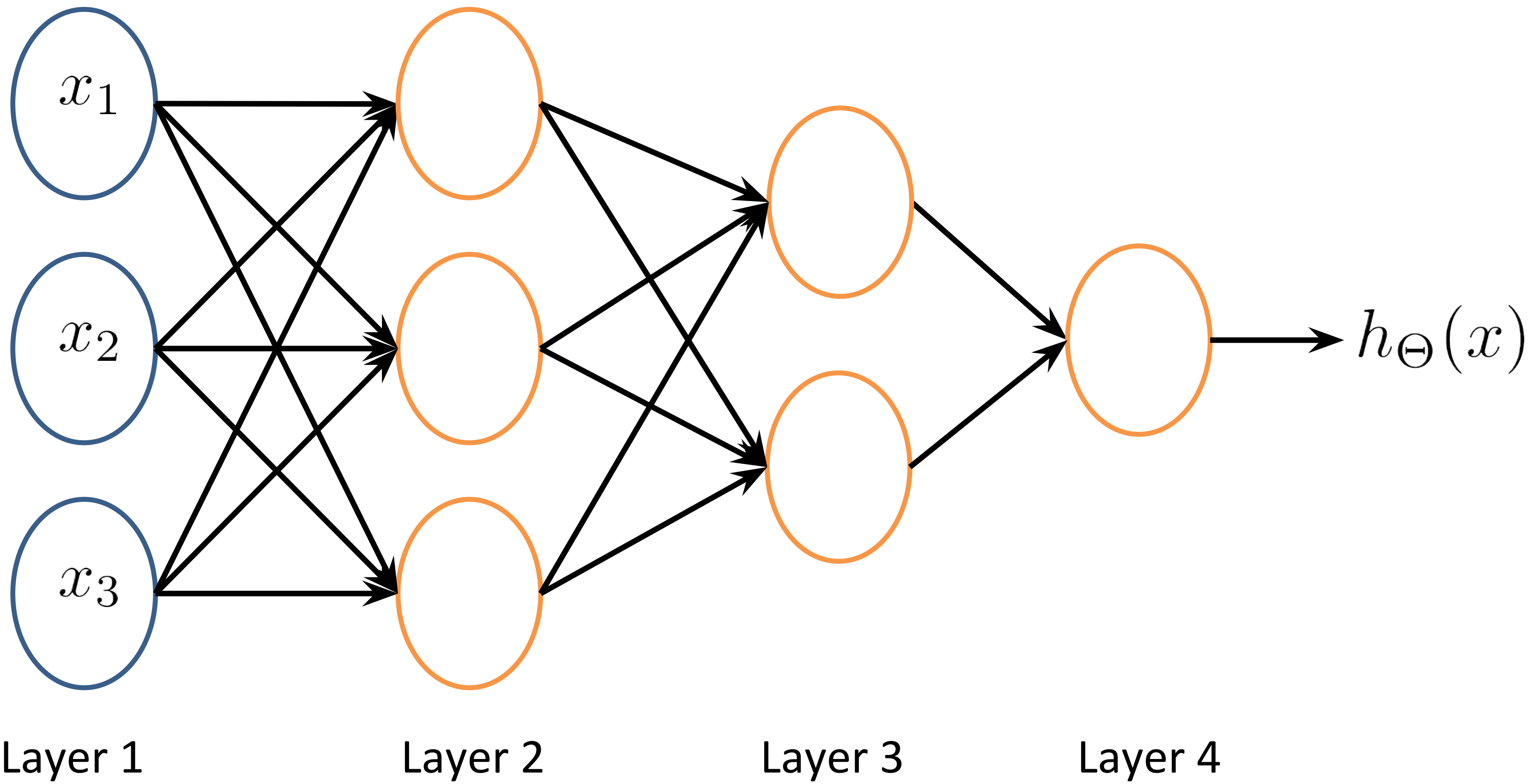
Add $a_0^{(2)} = 1$.

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

Neural Network learning its own features



Other network architectures

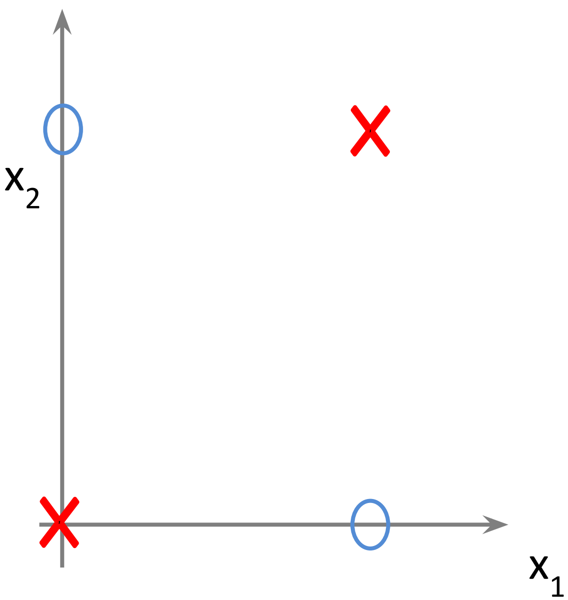


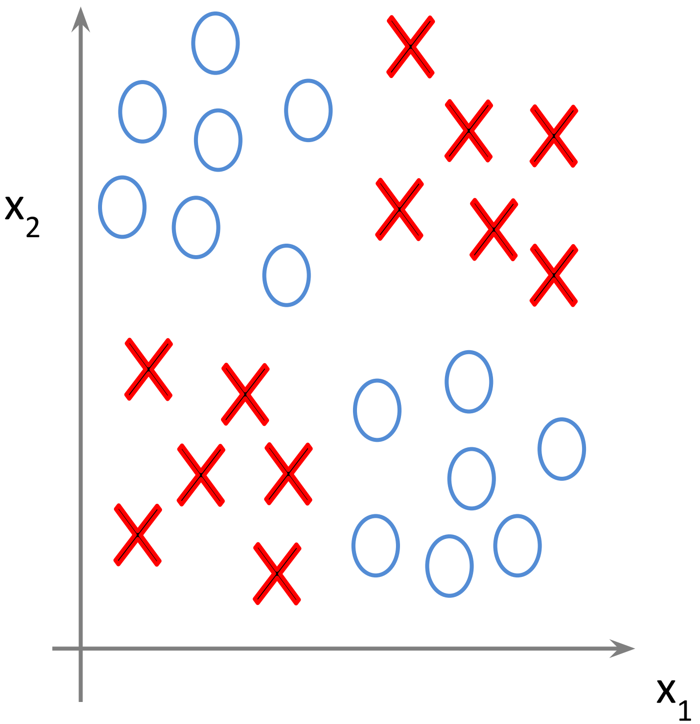
Neural Networks: Representation

Examples and intuitions I

Non-linear classification example: XOR/XNOR

x_1, x_2 are binary (0 or 1).





$$y = x_1 \text{ XOR } x_2$$

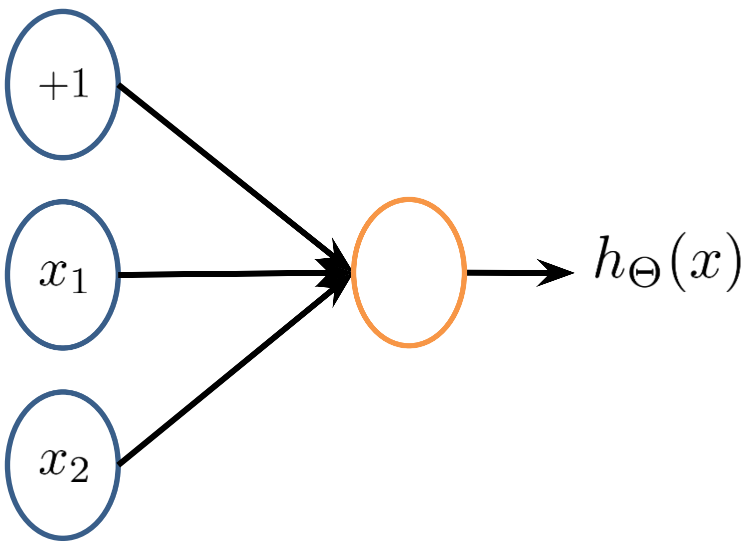
$$x_1 \text{ XNOR } x_2$$

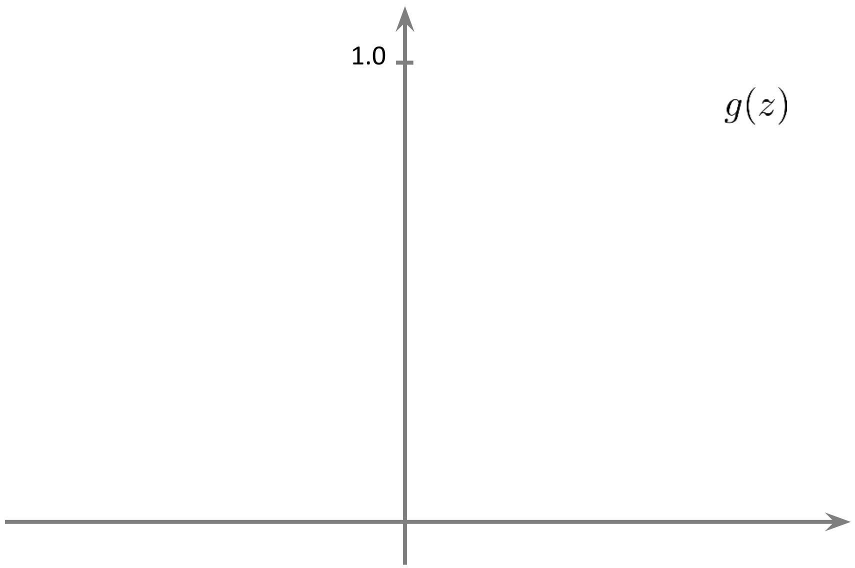
$$\text{NOT } (x_1 \text{ XOR } x_2)$$

Simple example: AND

$$x_1, x_2 \in \{0, 1\}$$

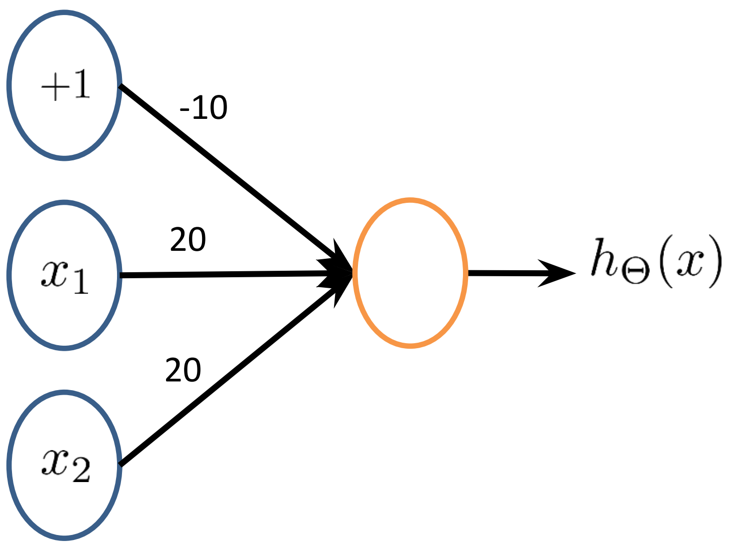
$$y = x_1 \text{ AND } x_2$$





x_1	x_2	$h_\Theta(x)$
0	0	
0	1	
1	0	
1	1	

Example: OR function



x_1	x_2	$h_\Theta(x)$
0	0	
0	1	
1	0	
1	1	

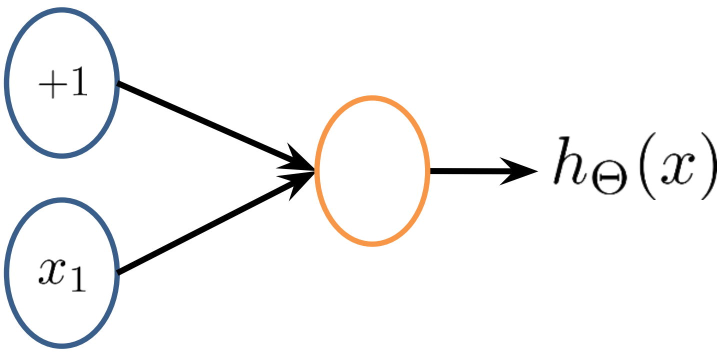
Neural Networks: Representation

Examples and intuitions II

Machine Learning

x_1 AND x_2 | x_1 OR x_2

Negation:

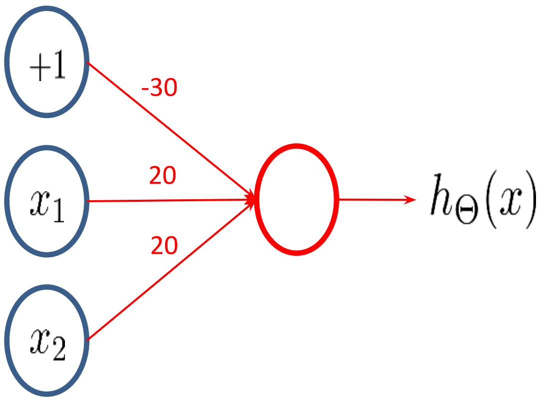


x_1	$h_\Theta(x)$
0	
1	

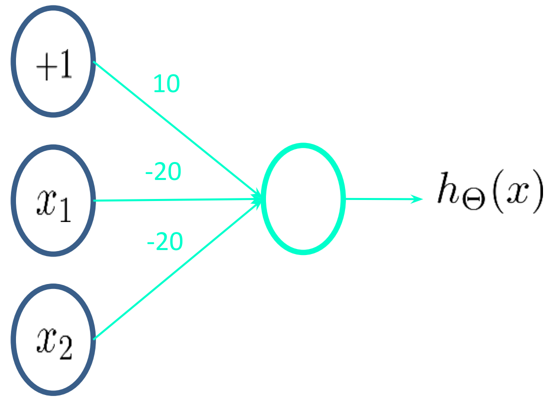
$$h_\Theta(x) = g(10 - 20x_1)$$

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

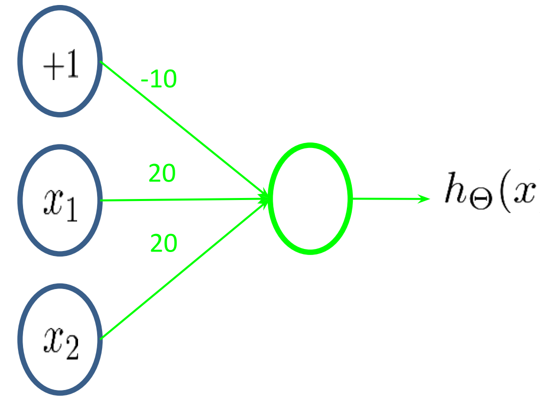
Putting it together: $x_1 \text{ XNOR } x_2$



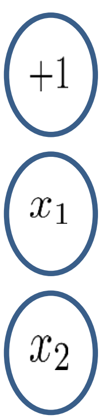
$x_1 \text{ AND } x_2$



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

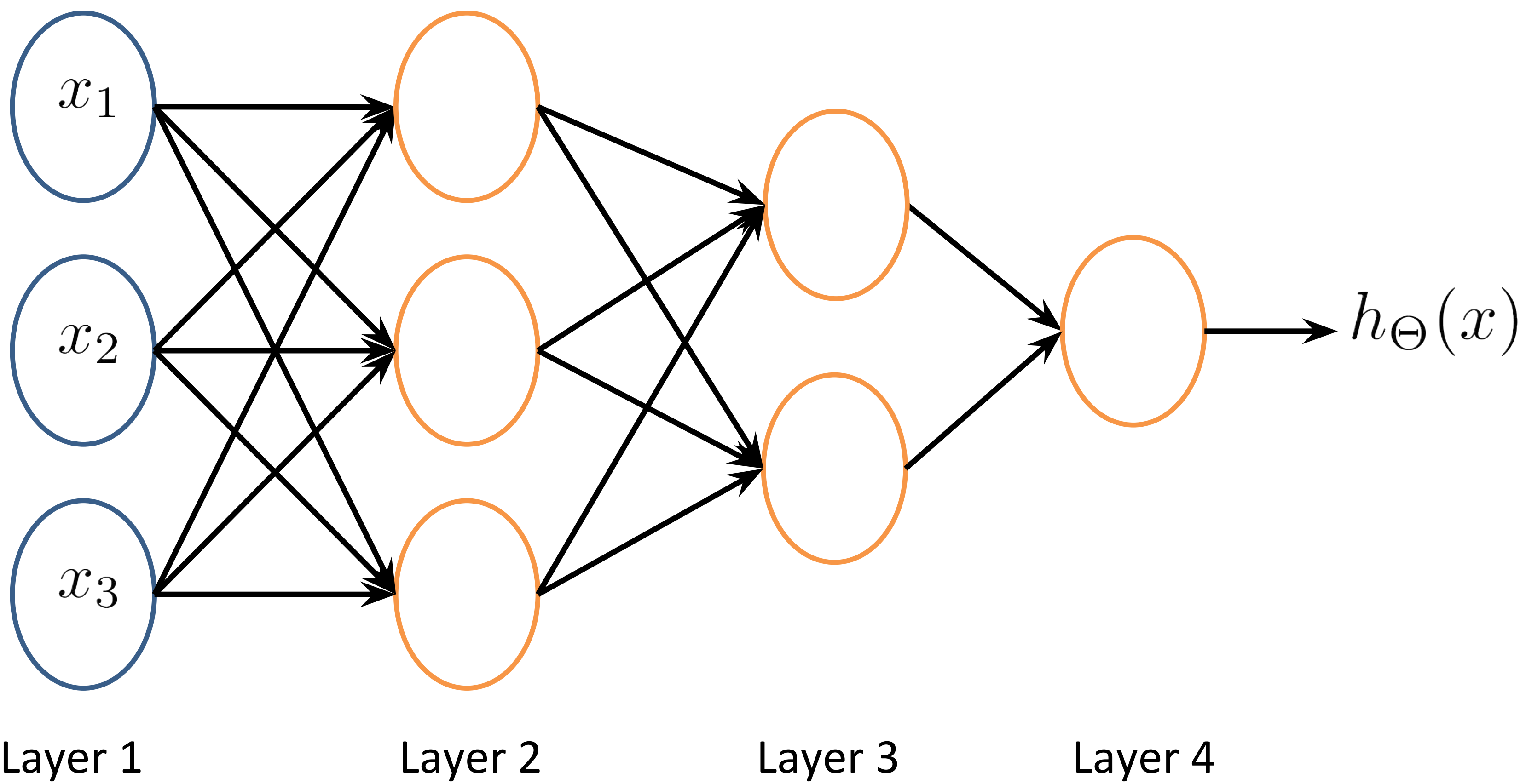


$x_1 \text{ OR } x_2$



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

Neural Network intuition



Handwritten digit classification

[Courtesy of Yann LeCun]

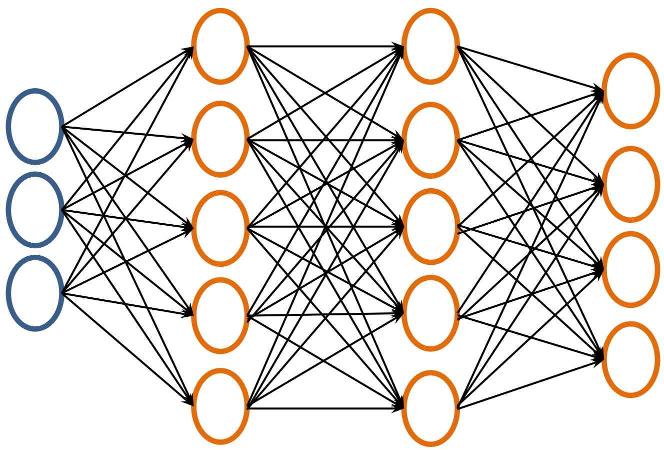
Multiple output units: One-vs-all.

Pedestrian

Car

Motorcycle

Truck

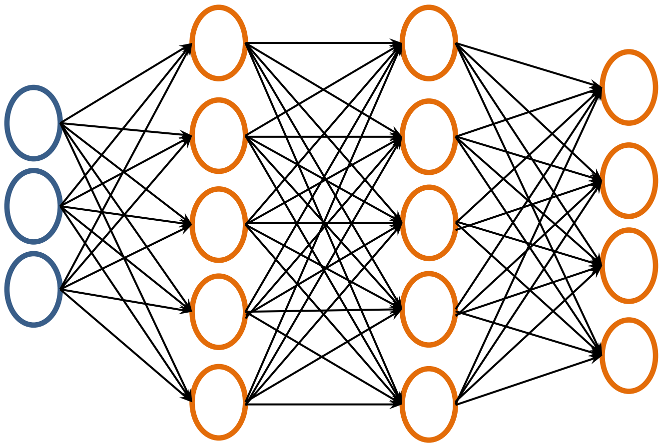


$$h_\Theta(x) \in \mathbb{R}^4$$

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

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

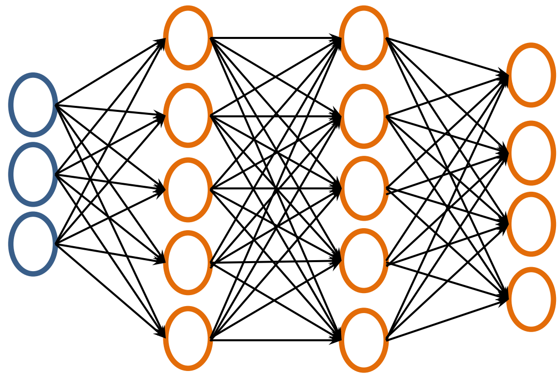
$y^{(i)}$ one of $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

pedestrian   car   motorcycle   truck

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

$y = 0 \text{ or } 1$

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

Backpropagation algorithm

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:

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

Gradient computation

Given one training example (x, y):

Forward propagation:

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

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

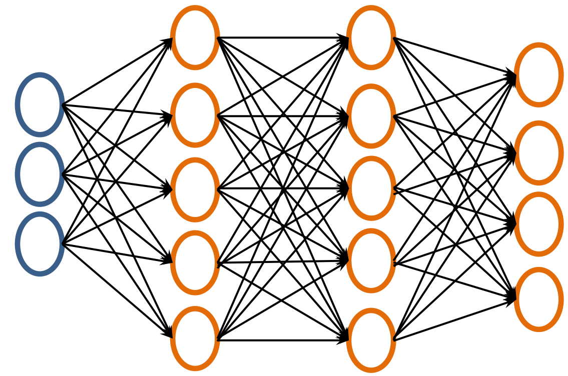
$$a^{(2)} = g(z^{(2)}) \quad (\text{add } a_0^{(2)})$$

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

$$a^{(3)} = g(z^{(3)}) \quad (\text{add } a_0^{(3)})$$

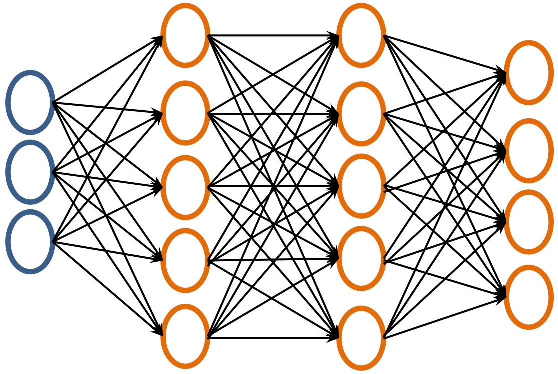
$$z^{(4)} = \Theta^{(3)} a^{(3)}$$

$$a^{(4)} = h_\Theta(x) = g(z^{(4)})$$



Gradient computation: Backpropagation algorithm

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



For each output unit (layer L = 4)

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

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

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

Backpropagation algorithm

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

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

For $i = 1 \text{ to } m$

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

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

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

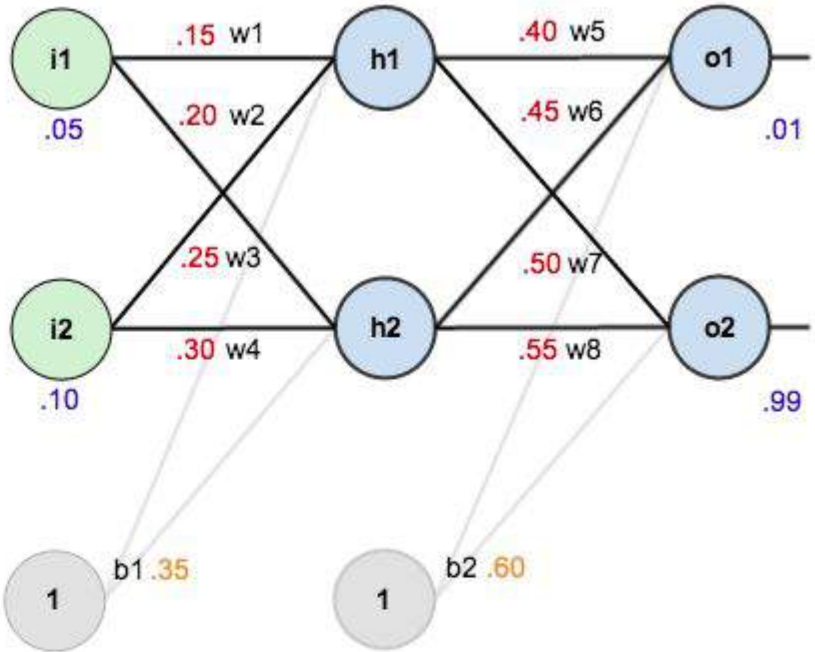
$$D_{ij}^{(l)} := \frac{1}{m} \triangle_{ij}^{(l)} + \lambda \Theta_{ij}^{(l)} \text{ if } j \neq 0$$

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

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

Neural Networks: Learning

Backpropagation intuition



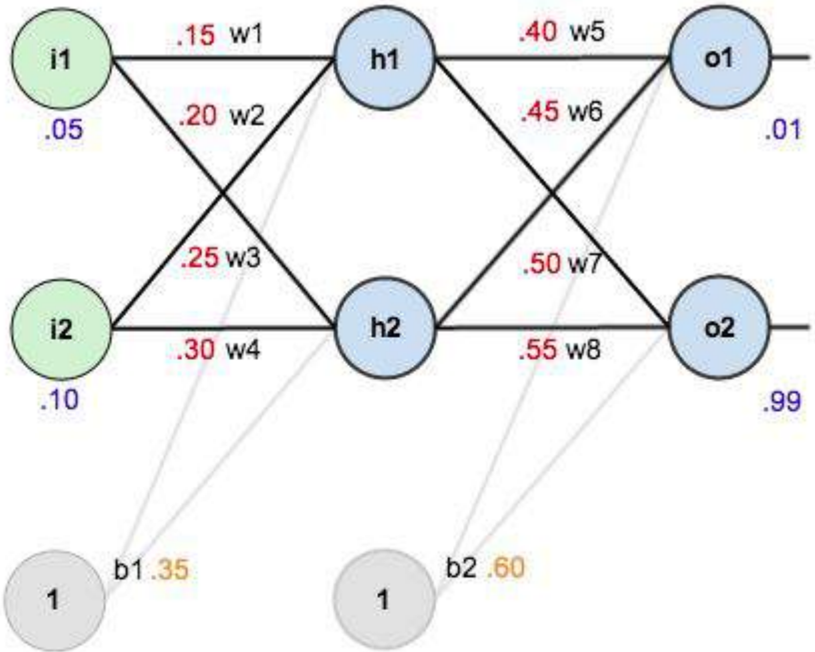
Forward Propagation

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

$$net_{h1} = 0.15 * 0.05 + 0.2 * 0.1 + 0.35 * 1 = 0.3775$$

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}} = \frac{1}{1+e^{-0.3775}} = 0.593269992$$

$$out_{h2} = 0.596884378$$

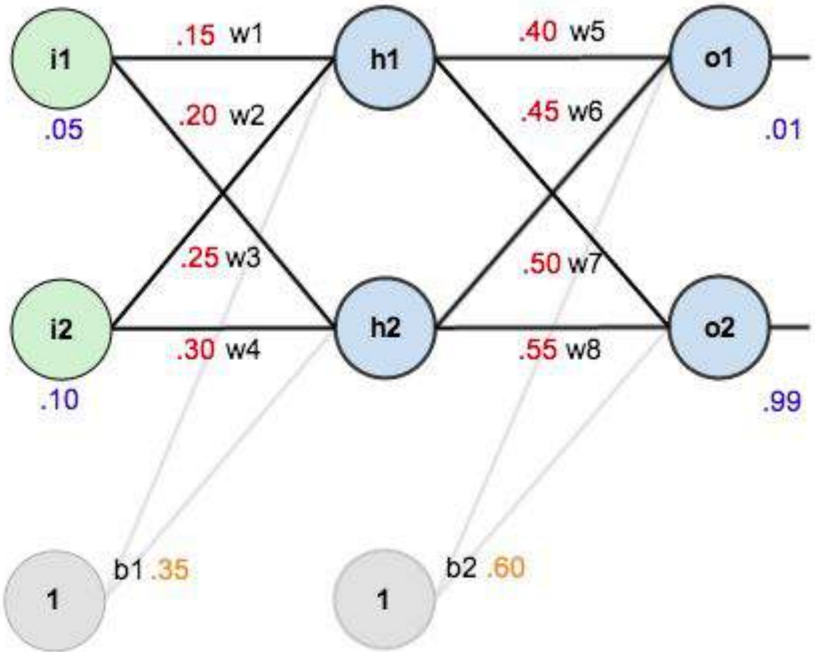


$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$net_{o1} = 0.4 * 0.593269992 + 0.45 * 0.596884378 + 0.6 * 1 = 1.105905967$$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}} = \frac{1}{1+e^{-1.105905967}} = 0.75136507$$

$$out_{o2} = 0.772928465$$



Calculating the Total Error

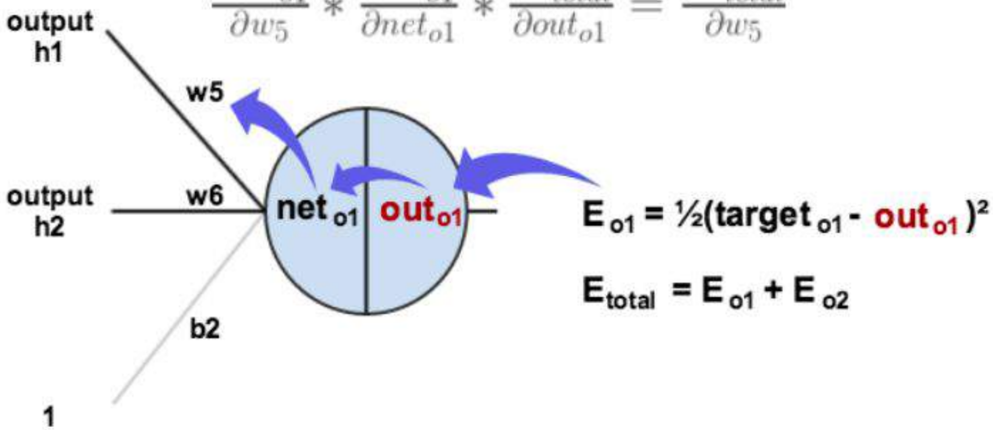
$$E_{total} = \sum \frac{1}{2}(target - output)^2$$

$$E_{o1} = \frac{1}{2}(target_{o1} - out_{o1})^2 = \frac{1}{2}(0.01 - 0.75136507)^2 = 0.274811083$$

$$E_{o2} = 0.023560026$$

$$E_{total} = E_{o1} + E_{o2} = 0.274811083 + 0.023560026 = 0.298371109$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



The Backwards Pass

$$E_{total} = \frac{1}{2}(target_{o1} - out_{o1})^2 + \frac{1}{2}(target_{o2} - out_{o2})^2$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = 2 * \frac{1}{2}(target_{o1} - out_{o1})^{2-1} * -1 + 0$$

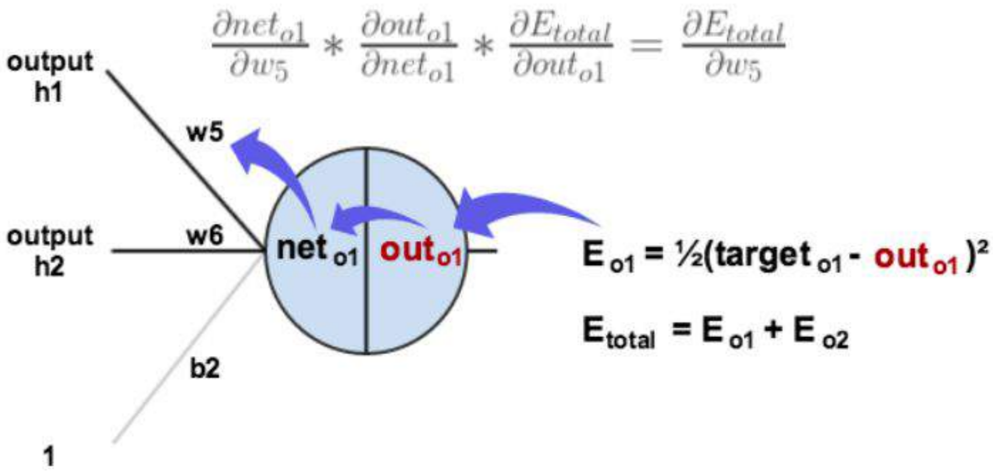
$$\frac{\partial E_{total}}{\partial out_{o1}} = -(target_{o1} - out_{o1}) = -(0.01 - 0.75136507) = 0.74136507$$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial net_{o1}} = out_{o1}(1 - out_{o1}) = 0.75136507(1 - 0.75136507) = 0.186815602$$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial net_{o1}} = out_{o1}(1 - out_{o1}) = 0.75136507(1 - 0.75136507) = 0.186815602$$



The Backwards Pass

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$

$$\frac{\partial E_{total}}{\partial w_5} = 0.74136507 * 0.186815602 * 0.593269992 = 0.082167041$$

$$w_5^+ = w_5 - \eta * \frac{\partial E_{total}}{\partial w_5} = 0.4 - 0.5 * 0.082167041 = 0.35891648$$

$$w_6^+ = 0.408666186$$

$$w_7^+ = 0.511301270$$

$$w_8^+ = 0.561370121$$

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}}$$