

Notes

Machine Learning by Andrew Ng on Coursera

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Contents

1	Introduction	3
1.1	Supervised Learning	3
1.1.1	Regression Problem	3
1.1.2	Classification Problems	3
1.2	Unsupervised Learning	3
2	Linear Regression with One Variable	4
2.1	Notations	4
2.2	Supervised Learning	4
2.3	Gradient Descent	5
2.4	Gradient Descent for Linear Regression	5
3	Linear Algebra	6
3.1	Matrix	6
3.2	Vector	6
3.3	Addition and Scalar Multiplication	7
3.4	Matrix Matrix Multiplication	7
3.5	Inverse and Transpose	7
4	Linear Regression with Multiple Variables	9
4.1	Notations	9
4.2	Hypothesis	9
4.3	Gradient Descent	10
4.3.1	Feature Scaling	10
4.3.2	Mean Normalization	11
4.3.3	Learning Rate	11
4.4	Features and Polynomial Regression	11
4.4.1	Features	11
4.4.2	Polynomial Regression	11
4.5	Normal Equation	12
4.5.1	Non Invertibility of $X^T X$	12

5	Octave Tutorial	13
6	Classification	14
6.1	Logistic Regression	14
6.2	Decision Boundary	15
6.3	Cost Function	15
6.4	Advanced Optimization:	17
6.5	Multi-Class Classification	18
6.5.1	One vs All	18
7	Regularization	19
7.1	Problem of Overfitting	19
7.2	Addressing Overfitting	19
7.3	Cost Function	20
7.4	Regularized Linear Regression	20
7.5	Regularized Logistic Regression	22
8	Neural Networks	23
8.1	Non-Linear Hypothesis	23
8.2	Neural Networks	23
8.3	Model Representation	23
8.4	Notations	24
8.5	Forward Propagation	25

Chapter 1

Introduction

Machine learning (task, experience, performance) can be classified into *Supervised* and *Unsupervised* learning.

1.1 Supervised Learning

Supervised learning can be basically classified into *Regression* and *Classification* problems.

1.1.1 Regression Problem

Regression problems work loosely on continuous range of outputs.

1.1.2 Classification Problems

Classification problems work loosely on discrete range of outputs.

1.2 Unsupervised Learning

An example is *Clustering Problem*.

Check Lecture1.pdf for more details.

Chapter 2

Linear Regression with One Variable

2.1 Notations

m = number of training examples

x 's = 'input' variables / features

y 's = 'output' variables / 'target' variables

(x, y) = single training example

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

2.2 Supervised Learning

We have a data set (*Training Set*).

Training Set \rightarrow Learning Algorithm $\rightarrow h$ (*hypothesis*, a function $X \rightarrow Y$)

To Represent h

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

Cost

$$\underset{\theta_0, \theta_1}{\text{minimize}} \frac{1}{2m} \sum_1^m (h_{\theta}(x) - y)^2$$

Cost Function

Squared Error Cost Function

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_1^m (h_{\theta}(x) - y)^2$$

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

2.3 Gradient Descent

Finds local optimum:

1. Start with some value
2. Get closer to optimum

Algorithm

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

where α = learning rate

Important!

Simultaneous Update!

$$\begin{aligned} temp_j &:= \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \quad \forall j \\ \theta_j &:= temp_j \quad \forall j \end{aligned}$$

2.4 Gradient Descent for Linear Regression

Cost function for linear regression is convex!

Batch Gradient Descent: Each step of gradient descent uses all training examples.

Check Lecture2.pdf for more details.

Chapter 3

Linear Algebra

3.1 Matrix

Rectangular array of numbers:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Dimension of the matrix: #rows x #cols (2 x 3)

Elements of the matrix:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

A_{ij} = “ i, j entry” in the i^{th} row, j^{th} col

3.2 Vector

An $n \times 1$ matrix.

$$y = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

$$y_i = i^{th} \text{ element}$$

Note: Uppercase for matrices, lowercase for vectors.

3.3 Addition and Scalar Multiplication

Add/Subtract (element by element) matrices of same dimension only!

Multiply/Divide (all elements) a matrix by scalar!

3.4 Matrix Matrix Multiplication

$m \times n$ matrix multiplied by $n \times o$ matrix gives a $m \times o$ matrix.

Properties

1. Matrix Multiplication is *not* Commutative.
2. Matrix Multiplication is Associative.
3. *Identity Matrix (I)*: 1's along diagonal, 0's everywhere else in an $n \times n$ matrix. $AI = IA = A$.

3.5 Inverse and Transpose

Inverse

Only square ($n \times n$) matrices *may* have an inverse.

$$AA^{-1} = A^{-1}A = I$$

Matrices that don't have an inverse are *singular* or *degenerate* matrices.

Transpose

Let A be an $m \times n$ matrix and let $B = A^T$, then

$$B_{ij} = A_{ji}$$

Example:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$
$$B = A^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

Check Lecture3.pdf for more details.

Chapter 4

Linear Regression with Multiple Variables

4.1 Notations

n = number of features

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

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

4.2 Hypothesis

Previously:

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

Now:

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

For convinience, define $x_0 = 1$. So

$$h_{\theta}(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

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

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

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

4.3 Gradient Descent

Hypothesis : $h_{\theta}(x) = \theta^T x$

Parameters : θ

$$= \theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_n x_n$$

$$= \theta_0, \theta_1, \dots, \theta_n$$

Cost Function : $J(\theta) = J(\theta_0, \theta_1, \dots, \theta_n)$

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

Gradient Descent :

Repeat{

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

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

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

} (simultaneously update $\forall j = 0, 1, \dots, n$)

4.3.1 Feature Scaling

Idea: Make sure features are on a similar scale.

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

4.3.2 Mean Normalization

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

General Rule

$$x_i \leftarrow \frac{x_i - \mu_i}{S_i}$$

where

μ_i = average value of x_i

S_i = range (max - min) *or*

= σ (standard deviation)

4.3.3 Learning Rate

$J(\theta)$ should decrease after every iteration. #iterations vary a lot.

Example *Automatic Convergence Test*: Declare convergence if $J(\theta)$ decreases by less than ϵ (say 10^{-3}) in one iteration.

If $J(\theta)$ increases, use smaller α . Too small α means slow convergence.

To choose α , try ..., 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1, ...

4.4 Features and Polynomial Regression

4.4.1 Features

Get an insight in your problem and choose better features (may even combine/separate features).

Ex: size = length \rightarrow breadth.

4.4.2 Polynomial Regression

Ex:

$$x_1 = size$$

$$x_2 = size^2$$

$$x_3 = size^3$$

4.5 Normal Equation

Solve for θ analytically!

$$\begin{aligned}x^{(i)} &= \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix} && \in \mathbb{R}^{n+1} \\X &= \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} && \in \mathbb{R}^{m \times (n+1)} \\&= \begin{bmatrix} x_0 & x_1 & \dots & x_n \end{bmatrix} && \in \mathbb{R}^{m \times (n+1)} \\y &= \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} && \in \mathbb{R}^m \\\theta &= (X^T X)^{-1} X^T y\end{aligned}$$

Inverse of a matrix grows as $O(n^3)$, use wisely.

4.5.1 Non Invertibility of $X^T X$

Use 'pinv' function in Octave (pseudo-inverse) instead of 'inv' function (inverse).

If $X^T X$ is non-invertible, common causes are

1. Redundant features (linearly dependent)
2. Too many features ($m \leq n$). In this case, delete some features or use *regularization*

Check Lecture4.pdf for more details.

Chapter 5

Octave Tutorial

Check Lecture5.pdf for more details.

Chapter 6

Classification

Classify into categories (binary or multiple).

6.1 Logistic Regression

$$\begin{aligned} 0 &\leq h_{\theta}(x) \leq 1 \\ h_{\theta}(x) &= g(\theta^T x) \\ g(z) &= \frac{1}{1 + e^{-z}} \quad g \text{ is called a } \textit{sigmoid} \text{ function or a } \textit{logistic} \text{ function.} \\ h_{\theta}(x) &= \frac{1}{1 + e^{\theta^T x}} \end{aligned}$$

Interpretation of Hypothesis Output

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

$h_{\theta}(x) = P(y = 1|x; \theta)$ = probability that $y = 1$, given x , parameterized by θ

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

6.2 Decision Boundary

$$\begin{array}{ll} \text{Predict: } y = 1 & \text{if } h_{\theta}(x) \geq 0.5 \\ & (\theta^T x \geq 0) \\ \text{Predict: } y = 0 & \text{if } h_{\theta}(x) < 0.5 \\ & (\theta^T x < 0) \\ \theta^T x = 0 & \text{is the } \textit{decision boundary}. \end{array}$$

Non-linear Decision Boundaries

Use same technique as polynomial regression for features.

6.3 Cost Function

Training Set : $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})\}$

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

$$x_0 = 1$$

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

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

How to choose parameter θ ?

Linear Regression:

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

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

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

Logistic Regression:

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

$$\text{Cost}(h_{\theta}(x), y) = 0 \text{ if } h_{\theta}(x) = y$$

$$\text{Cost}(h_{\theta}(x), y) \rightarrow \inf \text{ if } y = 0 \text{ and } h_{\theta}(x) \rightarrow 1$$

$$\text{Cost}(h_{\theta}(x), y) \rightarrow \inf \text{ if } y = 1 \text{ and } h_{\theta}(x) \rightarrow 0$$

Note: $y = 0$ or 1 always.

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

$$\begin{aligned} J(\theta) &= \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_{\theta}(x^{(i)}), y^{(i)}) \\ &= -\frac{1}{m} \left[\sum_{i=1}^m (y^{(i)} \log(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)}))) \right] \end{aligned}$$

To fit parameters θ :

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

To make a prediction given a new x :

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

Gradient Descent:

Simultaneously update all θ_j

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

Plug in the derivative

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

Don't forget feature scaling!

6.4 Advanced Optimization:

Something better than gradient descent:

1. Conjugate Gradient
2. BFGS
3. L-BFGS

Advantages:

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

Disadvantages:

1. More complex

Use libraries! Beware of bad implementations!

How to use: We first need to provide a function that evaluates the following two functions for a given input value of θ .

1. $J(\theta)$
2. $\frac{\partial}{\partial \theta_j} J(\theta)$

```

% We can write a single function that can return both of these:
function [jVal, gradient] = costFunction(theta)
    jVal = [...code to compute J(theta)...];
    gradient = [...code to compute derivative of J(theta)...];
end

```

Then we can use octave's *fminunc()* optimization algorithm along with the *optimset()* function that creates an object containing the options we want to send to *fminunc()*.

```

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

```

6.5 Multi-Class Classification

6.5.1 One vs All

Build a separate binary classifier $h_{\theta}^{(i)}(x)$ for each class against all other classes.

$$h_{\theta}^{(i)} = P(y = i|x; \theta) \quad \forall i$$

On a new input x , to make a prediction, pick the class i that maximizes $h_{\theta}^{(i)}(x)$

Check Lecture6.pdf for more details.

Chapter 7

Regularization

7.1 Problem of Overfitting

1. Underfitting (High Bias)
2. Right Fit
3. Overfitting (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).

7.2 Addressing Overfitting

Options:

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

7.3 Cost Function

Say our overfitting hypothesis is $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$. Suppose, we penalize and make θ_3, θ_4 very small

$$\underset{\theta}{\text{minimize}} \left(\frac{1}{2m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})^2 + 1000\theta_3^2 + 1000\theta_4^2 \right)$$

Regularization

Small values for parameters $\theta_0, \theta_1, \dots, \theta_n$.

- *Simpler* hypothesis
- Less prone to overfitting

Which parameters to penalize?

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

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

Note: The convention, we don't regularize θ_0 but it doesn't make very much difference.

λ here is *regularization parameter*.

What if λ is set too high (say 10^{10})? Underfitting!

7.4 Regularized Linear Regression

Updated $J(\theta)$:

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

Gradient Descent:

Repeat{

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

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^m \left((h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right] \quad \forall j \in \{1, 2, \dots, n\}$$

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

}

Normal Equation:

$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \in \mathbb{R}^{m \times (n+1)}$$

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

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

Non-Invertibility

Suppose $m \leq n$,

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

If $\lambda > 0$,

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

Not a problem!

7.5 Regularized Logistic Regression

Cost Function:

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

Gradient Descent:

Repeat{

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

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^m ((h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}) + \frac{\lambda}{m} \theta_j \right] \quad \forall j \in \{1, 2, \dots, n\}$$

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

}

Advanced Optimization:

```
function [jVal, gradient] = costFunction(theta)
    jVal = [...code to compute J(theta)...];
    gradient = [...code to compute derivative of J(theta)...];
```

Check Lecture7.pdf for more details.

Chapter 8

Neural Networks

8.1 Non-Linear Hypothesis

If #features is high, hypothesis could have extremely high #terms. Hence the need for non-linear hypothesis.

8.2 Neural Networks

- *Origins:* Algorithms that try to mimic brain.
- Widely used in 80s and early 90s; diminished in late 90s.
- Resurgence: State-of-the-art technique for many applications.

8.3 Model Representation

Neuron Model: Logistic Unit

1. input layer
2. hidden layer / computation layer
3. output layer
4. activation function ($g()$)

parameters \equiv weights

8.4 Notations

$a_i^{(j)}$ = *activation* of unit i in layer j
 $\Theta^{(j)}$ = matrix of weights controlling
 function mapping from layer j to
 layer $j + 1$

Example:

layer 1 : $\{x_1, x_2, x_3\}$

layer 2 : $\{a_1^{(2)}, a_2^{(2)}, a_3^{(2)}\}$

layer 3 : $\{a_1^{(3)}\}$

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

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

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

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

Note: If network has s_j units in layer j , and s_{j+1} units in layer $j + 1$, then

$$\Theta^{(j)} \in \mathbb{R}^{s_{j+1} \times (s_j + 1)}$$

8.5 Forward Propagation

$$z_1^{(2)} = \Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3$$

$$z_2^{(2)} = \Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3$$

$$z_3^{(2)} = \Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3$$

$$a_1^{(2)} = g(z_1^{(2)})$$

$$a_2^{(2)} = g(z_2^{(2)})$$

$$a_3^{(2)} = g(z_3^{(2)})$$

Vectorized Implementation

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad x_0 = 1$$

$$z^{(2)} = \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix}$$

$$a^{(1)} = x \quad \in \mathbb{R}^4$$

$$z^{(2)} = \Theta^{(1)} a^{(1)} \quad \in \mathbb{R}^3$$

$$a^{(2)} = g(z^{(2)}) \quad \in \mathbb{R}^3$$

$$\text{Add } a_0^{(2)} = 1 \quad \rightarrow a^{(2)} \in \mathbb{R}^4$$

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

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

Other network architectures are possible!