

Week 3

Classification

Classification is similar to regression, just that there are a smaller number of discrete values instead of real values

Ex:

Email: Spam / Not Spam?

Online transaction: Fraudulent (Yes/No)?

Tumor: Malignant / Benign?

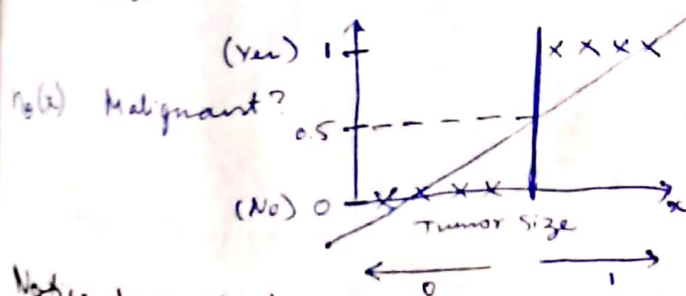
$y \in \{0, 1\}$ 0: Negative class (eg. benign tumor)
1: Positive class (eg. malignant tumor)

Binary classification (Only 2 classes - 0 & 1)

$y \in \{0, 1, 2, \dots\} \in$ Multiclass classification

Problem with applying linear regression to classification problem

We can map all predictions > 0.5 as 1 and < 0.5 as 0.



Notice how that point changes the linear regression line, due to which 2 data points are classified wrong

We cannot use linear regression for classification problem. So we use

Logistic Regression

If $h_0(x) \geq 0.5$, predict $y=1$
If $h_0(x) < 0.5$, predict $y=0$

Suppose we add a new data point here. Then it gets screwed

Here $h_0(x) > 0.5$ and $h_0(x) < 0$ but y should $\in \{0, 1\}$ so this doesn't make sense. We need $0 \leq h(x) \leq 1$

Logistic Regression

- we need to plot a better curve that fits the data better
- $0 \leq h_\theta(x) \leq 1$ since $y \in (0, 1)$

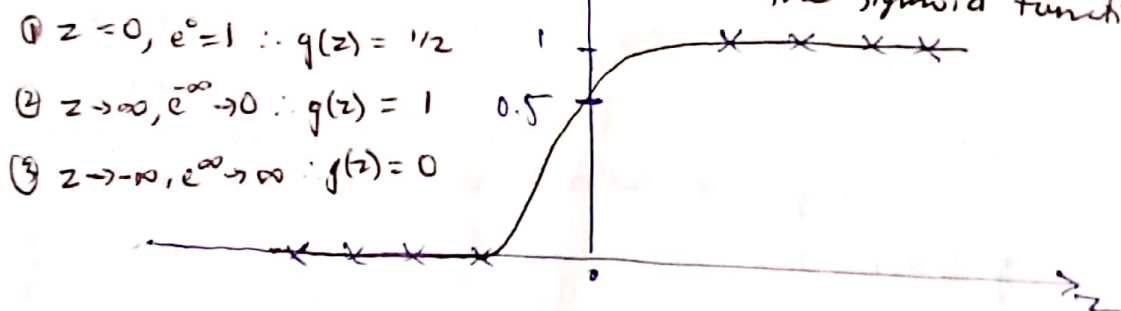
∴ We use the Sigmoid Function (also called Logistic Function)

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

Let $z = \theta^T x$,

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

hypothesis function
in vector form
on which we apply
the sigmoid function



$h_\theta(x)$ will be probability that our output is 1

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

Probability of $y=1$ given x
parameterized by θ

Exa:

If $h_\theta(x) = 0.7$ in tumor example, it means the patient has a 70% probability of having a malignant tumor ($y=1$).

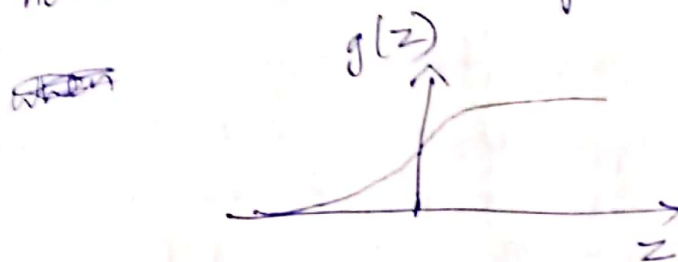
The probability of having a benign tumor is $1 - 0.7 = 0.3$ ∴ 30%.

Decision Boundary

In order to get discrete 0 or 1 classification, we can translate the output of the hypothesis function as follows,

$$h_\theta(x) \geq 0.5 \rightarrow y = 1$$

$$h_\theta(x) < 0.5 \rightarrow y = 0$$



From the diagram,

$$\text{When } z \geq 0, g(z) \geq 0.5$$

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

$$\text{since } z = \theta^T x,$$

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

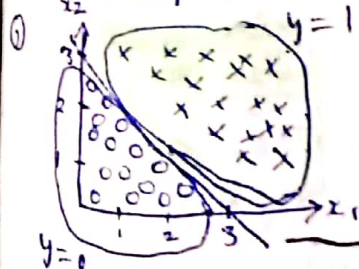
$$\text{or } \theta^T x \geq 0$$

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

$$\text{or } \theta^T x < 0$$

Decision boundary is the line that separates the area where $y=0$ and $y=1$. It is created by the hypothesis function.

Example



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

$$\text{let } \theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix} \text{ i.e. } \theta_0 = -3, \theta_1 = 1, \theta_2 = 1$$

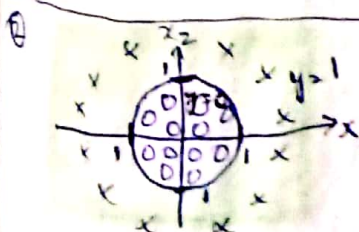
$$\therefore \text{Predict } y=1 \text{ if } -3 + x_1 + x_2 \geq 0$$

$$\text{equation of Line} \rightarrow x_1 + x_2 \geq 3$$

(Decision boundary)

At these points

$$h_\theta(x) = 0.5$$



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

$$\theta = \begin{bmatrix} -1 \\ 1 \\ 1 \\ 0 \end{bmatrix} \therefore \text{Predict } y \text{ if } -1 + x_1^2 + x_2^2 \geq 0$$

$$\text{equation of circle of radius 1} \rightarrow x_1^2 + x_2^2 \geq 1$$

Logistic Regression Model

Cost Function

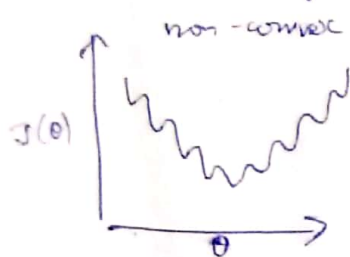
For linear regression $J(\theta) = \frac{1}{n} \sum_{i=1}^m \left(\frac{1}{2} (h_{\theta}(x^{(i)}) - y^{(i)})^2 \right)$

The cost the learning algorithm

needs to pay if it predicted $h_{\theta}(x^{(i)})$ instead of y .
cost $(h_{\theta}(x^{(i)}), y)$

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

Since we are using a logistic function for $h_{\theta}(x)$, we will get a non-convex function for the cost function if we try to use this for logistic regression.

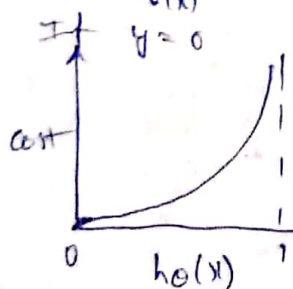
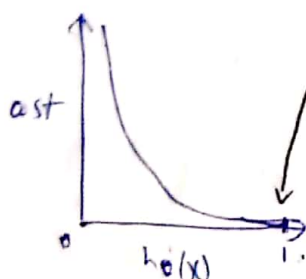


- Since $\frac{1}{1+e^{-\theta^T x}}$ is non-linear this happens

Therefore we will use the following cost function:

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

If $y=1$



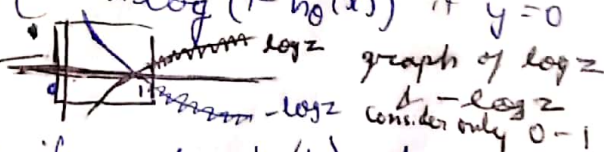
Cost = 0 if $y=1, h_{\theta}(x)=1$

As $h_{\theta}(x) \rightarrow 0$, Cost $\rightarrow \infty$

- as at 0 since if $y=1$ & it predicts $h_{\theta}(x)=0$, we need to penalise it by a very large cost

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

As $h_{\theta}(x) \rightarrow 1$, Cost $\rightarrow \infty$



Simplified Cost Function

$$\text{cost}(h_0(x), y) = \begin{cases} -\log(h_0(x)) & \text{if } y=1 \\ -\log(1-h_0(x)) & \text{if } y=0 \end{cases}$$

Combine the two cases in one equation,

$$\text{cost}(h_0(x), y) = -y \log(h_0(x)) - (1-y) \log(1-h_0(x))$$

$$\text{if } y=1, \text{cost}(h_0(x), y) = -\log(h_0(x)) - \cancel{0 \cdot \log(1-h_0(x))}$$

$$\text{if } y=0, \text{cost}(h_0(x), y) = -\log(1-h_0(x)) - \cancel{0 \cdot \log(h_0(x))}$$

Logistic Regression Cost Function

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m \text{cost}(h_0(x^{(i)}), y^{(i)})$$

$$= -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log(h_0(x^{(i)})) + (1-y^{(i)}) \log(1-h_0(x^{(i)})) \right]$$

Gradient Descent

Repeat $\{$

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \quad (\text{simultaneously update all } \theta_j)$$

$\}$

$$\text{Here } \frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_0(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

\therefore Repeat $\{$

$$\theta_j := \theta_j - \alpha \sum_{i=1}^m (h_0(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

$\}$

This algorithm looks identical to linear regression however note that here $h_0(x^{(i)}) = \frac{1}{1 + e^{-\theta^T x}}$

instead of $\theta^T x$

Vectorised implementation:

$$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \bar{y})$$

We can use feature scaling in logistical regression too to make gradient descent converge faster

Advanced Optimization

Apart from gradient descent, there are other advanced optimization functions:

- Conjugate Gradient
- BFGS
- L-BFGS

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

Disadvantages: - More complex

Example

$$\theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \quad J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$$

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

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

Here $\min J(\theta)$ is at $\theta_1 = 5, \theta_2 = 5$

We find this now:

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

$$jVal = (\text{theta}(1) - 5)^2 + (\text{theta}(2) - 5)^2;$$

$$\text{gradient} = \text{zeros}(2, 1);$$

$$\text{gradient}(1) = 2 * (\text{theta}(1) - 5);$$

$$\text{gradient}(2) = 2 * (\text{theta}(2) - 5);$$

```
options = optimset('GradObj', 'on', 'MaxIter', '100');
```

```
initialTheta = zeros(2, 1);
```

```
[optTheta, functionVal, exitFlag]
```

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

optTheta - values of θ

functionVal - value of $J(\theta)$ at $\min J(\theta)$ \rightarrow Should be 0

exitFlag - 1 - mean converged
0 - not converged

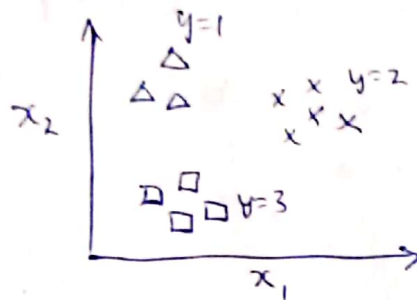
Multi-class Classification

When there are multiple classes

eg. Email foldering/tagging: $y=1$ Work, $y=2$ Friends, $y=3$ Family, $y=4$ Hilly

Medical diagnosis: Not ill, Cold, Flu

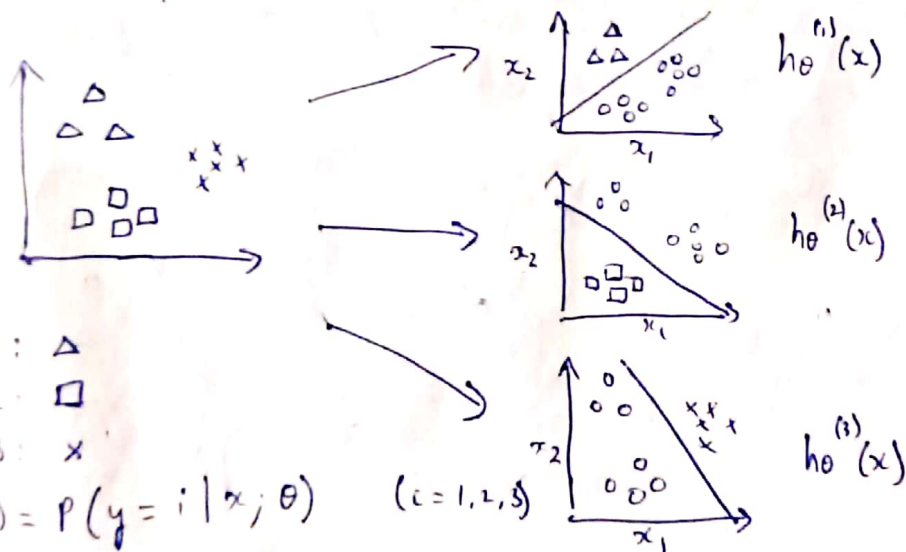
Weather: Sunny, Cloudy, Rain, Snow



$$y \in \{0, 1, 2, \dots, n\}$$

We can classify into different classes using

One-vs-all / One-vs-rest Method



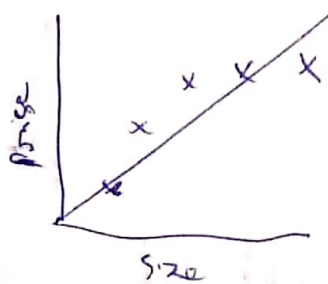
We choose one class and then lump all the others into a single second class. We do this repeatedly, applying binary logistic regression to each case, and then use the hypothesis that returned the highest value as our prediction.

$$\begin{aligned} h_0^{(0)}(x) &= P(y=0 | x; \theta) \\ h_0^{(1)}(x) &= P(y=1 | x; \theta) \\ &\vdots \\ h_0^{(n)}(x) &= P(y=n | x; \theta) \\ \text{prediction} &= \max_i (h_0^{(i)}(x)) \end{aligned}$$

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 generalise to new examples (predict prices on new examples)

Linear Regression (housing prices)

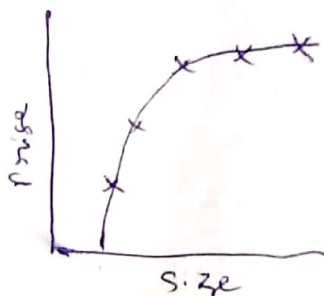


$$\theta_0 + \theta_1 x$$

Underfitting

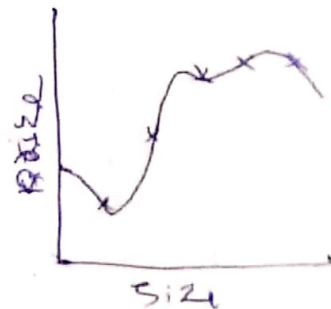
High bias

Doesn't fit training data well



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

Has a preconception or bias that the price will increase linearly even though data doesn't agree

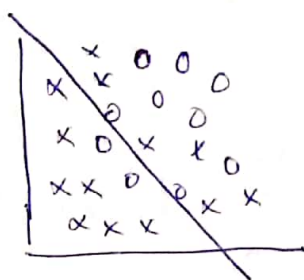


$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Overfitting

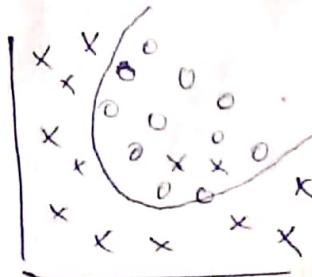
High variance

Logistic regression



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

Underfitting



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



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

overfitting

Addressing overfitting

1. Reduce no. of features
 - Manually select which features to keep
 - Model selection algorithm
2. Regularization
 - keep all features, but reduce magnitude values of θ_i
 - works well when we have a lot of features, each contributing a bit to predicting y .

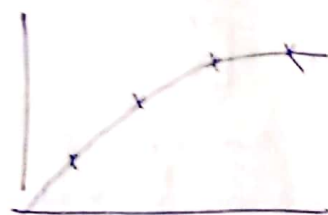
Regularisation

suppose we have overfitting



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

If we eliminate the influence of $\theta_3 x^3$ & $\theta_4 x^4$ we get a quadratic function $\theta_0 + \theta_1 x + \theta_2 x^2$ that fits our data well



we modify our cost function to

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

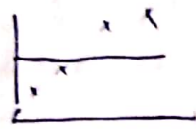
Here we have added 2 extra terms to inflate the cost of θ_3 & θ_4 . So for the cost function to get close to 0, we have to reduce θ_3 & θ_4 to 0, and this will reduce $\theta_3 x^3$ & $\theta_4 x^4$ in the ~~equation~~ ^{hypothesis} function.

Similarly we regularise all our θ parameters,

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

where λ - regularization parameter this is θ_j^2 square

Note: If λ is too large, it can result in underfitting since all the θ values are reduced essentially making the hypothesis function $h(x^{(i)}) = \theta_0$.



Note: we don't penalise θ_0 . Here j is from 1 to n

Regularized Linear Regression

Gradient descent:

Repeat {

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

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

$j \in \{1, 2, \dots, n\}$

}

Note that we took θ_0 separately since it's not regularised

If we take θ_j common for the second equation,

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

Here $(1 - \alpha \frac{\lambda}{m})$ will be less than 1. Intuitively we can see the equation as same as normal gradient descent but θ_j is reduced by some amount (e.g. $0.99\theta_j$) every iteration.

Normal equation:

$$\theta = (X^T X + \lambda \cdot L)^{-1} X^T y$$

where $L = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$ $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$

So for $n=2$, $(n+1) \times (n+1)$

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

Before we had a problem with the normal equation $(X^T X)^{-1} X^T y$

Here if $\underset{\substack{\uparrow \\ \text{no. of training examples}}}{m} > \underset{\substack{\uparrow \\ \text{no. of features}}}{n}$, then $X^T X$ would be non-invertible

However $(X^T X + \lambda \cdot L)$ makes it invertible and solves this problem.

Regularized Logistic regression

$$\text{Cost Function: } J(\theta) = - \left[\frac{1}{m} \sum_{i=1}^m y^{(i)} \log(h_\theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)})) \right]$$

Gradient descent:

$$+ \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2 \quad \leftarrow \text{This is square from } \theta_1, \theta_2, \dots \text{ Not } \theta_0$$

← same derivation,
Repeat {

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

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

}

only difference is that $h_\theta(x^{(i)}) = \frac{1}{1 + e^{-\theta^T x}}$ here

Advanced optimization:

function [val, gradient] = costFunction(theta)

val = [code to compute $J(\theta)$];

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

$$\text{gradient}(1) = [\text{code to compute } \frac{\partial}{\partial \theta_0} J(\theta)];$$
$$\frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\text{gradient}(2) = [\text{code to compute } \frac{\partial}{\partial \theta_1} J(\theta)];$$
$$\left(\frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)} \right) + \frac{\lambda}{m} \theta_1$$

$$\text{gradient}(3) = [\text{code to compute } \frac{\partial}{\partial \theta_2} J(\theta)];$$
$$\left(\frac{1}{m} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_2^{(i)} \right) + \frac{\lambda}{m} \theta_2$$

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

This is same as before but we have updated the equation to add the regularisation term. We later put this into function

function [costFunction, initialTheta, options];