Overfitting

There are two ways that our model can end up not performing well:

- Underfit / High Bias
- Overfit / High Variance

Overfitting occurs if we have too many features and the learnt hypothesis fits the training set too well and may even turn out to be 0 or close to 0, but fail to generalize new examples

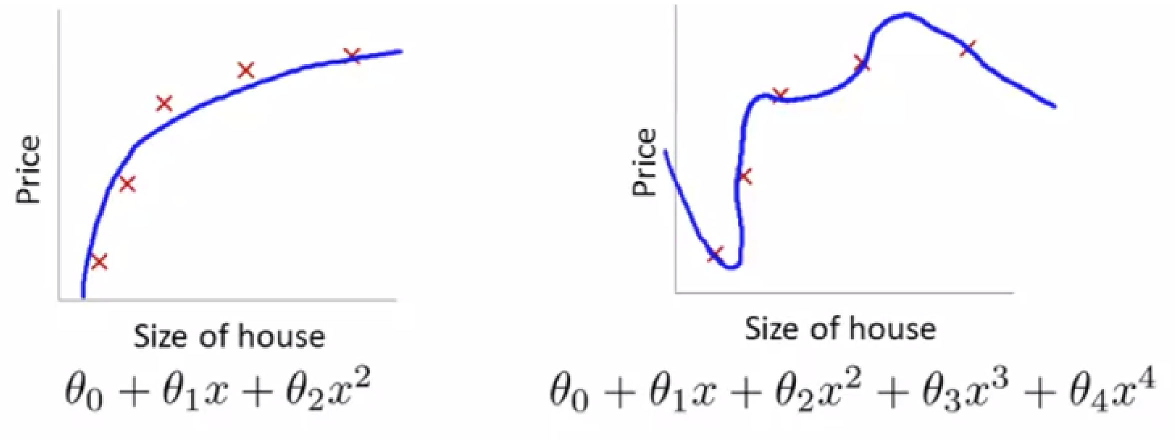
$$J(\theta) = \frac{1}{2m} \sum_{i=1} *m(h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$$

> Consider the medical diagnosis problem of classifying tumours as malignant or benign. If a hypothesis has overfit the training set, it means that:
>
> - [ ] It makes accurate predictions for examples in the training set and generalizes well to make accurate predictions on new, previously unseen examples
> - [ ] It does not make accurate predictions for examples in the training set, but it does generalize well to make accurate predictions on new, previously unseen examples
> - [x] It makes accurate predictions for examples in the training set, but it does not generalize well to make accurate predictions on new, previously unseen examples
> - [ ] It does not make accurate predictions for examples in the training set and does not generalize well to make accurate predictions on new, previously unseen examples.

Addressing Overfitting

- Reduce Number of Features
  - Manually select which features to keep
  - Model Selection Algorithm
- Regularization
  - Keep all the features, but reduce magnitude or values of parameters θ
  - Works well when we have a lot of features, each of which contributes a bit to predicting y

Cost Function Intuition



Suppose that we penalize and make θ_3 and θ_4 really small,

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

Now, let's modify the above objective and create a new one,

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

We'll end up with $\theta_3 \approx 0$ and $\theta_4 \approx 0$, which will essentially be a quadratic function.

Regularized Linear Regression

If we have small values for the parameters $\theta_0, \theta_1, \cdots, \theta_n$

- We end up with a simpler hypothesis
- Our model will be less prone to overfitting

Our cost function will be as follows:

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

Here, $\lambda = \text{Regularization Parameter}$. It controls the trade-off between the goal of fitting the training set well and the goal of keeping the parameters small.

> What if λ is set to an extremely large value (perhaps too large for our problem, say $\lambda = 10^{10}$?
>
> - Algorithm works fine
> - Algorithm fails to eliminate overfitting
> - Algorithm results in underfitting (fails to fit even the training set)
> - Gradient descent will fail to converge

Gradient Descent

repeat {

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

$$\theta_j := \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)} + \frac{\lambda}{m} \cdot \theta_j \right] \qquad (j = 1, 2, 3, \cdots, n)$$

}

To simplify the above, we can rewrite it as follows:

repeat {

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

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \frac{\alpha}{m} \cdot \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x_j^{(i)} \qquad (j = 1, 2, 3, \cdots, n)$$

}

Here $(1 - \alpha \frac{\lambda}{m}) < 1$

Normal Equation

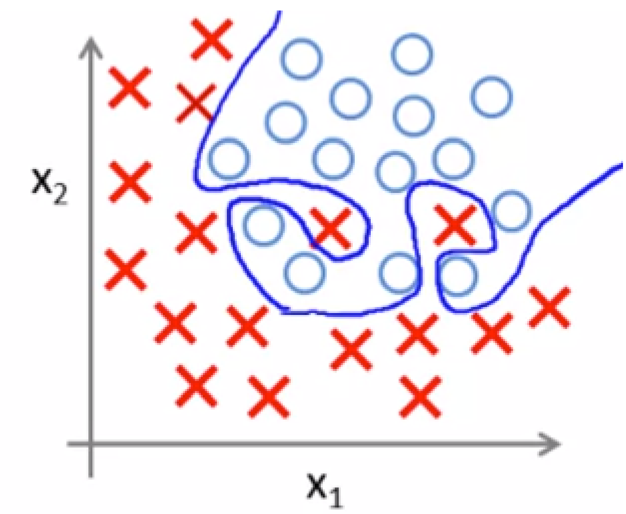
$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix}_{m*(n+1)} \qquad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

Objective is to $\min_\theta J(\theta)$

Where,

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

Regularized Logistic Regression



Suppose we have our hypothesis as:

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

Our cost function will be:

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

Gradient Descent

repeat {

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

$$\vdots$$

$$\theta_j := \theta_j - \alpha\left[\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j\right] \qquad [j = 1, 2, 3, \cdots, n]$$

}

Advanced optimization

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

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

```
    gradient(1) = [code to compute ∂/∂θ0 J(θ) ] ;
```

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

```
    gradient(2) = [code to compute ∂/∂θ1 J(θ) ] ;
```

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

```
    gradient(3) = [code to compute ∂/∂θ2 J(θ) ] ;
```

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

$$\vdots$$

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