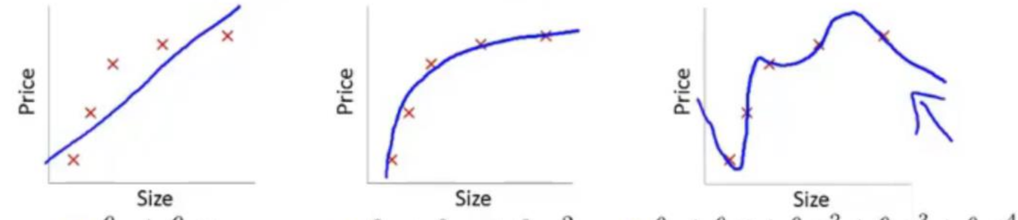
Regularization

1. The problem of overfitting

Example: Linear regression (housing prices)



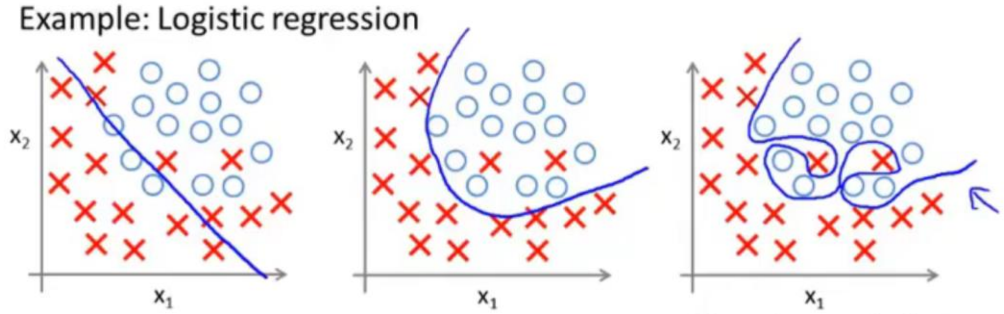
$\theta_0 + \theta_1 x$ "Underfit" "High bias"

$\theta_0 + \theta_1 x + \theta_2 x^2$ "Just right"

$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$ "Overfit" "High variance"

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

Example: Logistic regression



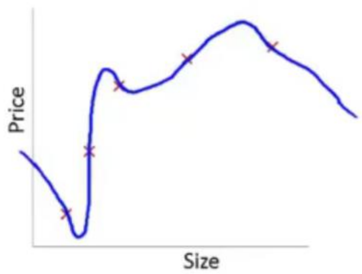
$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$
(g = sigmoid function)
"Underfit"

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

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

Addressing overfitting:

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



Addressing overfitting:

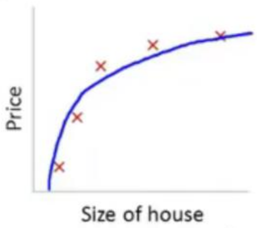
Options:

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

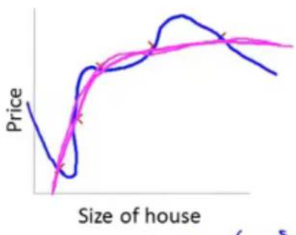
Andrew Ng

2. Cost function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

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

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

Regularization.

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

$\rightarrow \boxed{\theta_3, \theta_4} \approx 0$

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

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

$\cancel{\theta_0}$ $\theta_1, \theta_2, \theta_3, \ldots, \theta_{100}$ $\quad \cancel{\theta_0}$

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 $\lambda = 10^{10}$)?

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

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

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

$\boxed{h_\theta(x) = \theta_0}$

$h_\theta(x)$

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

3. Regularized linear regression

Regularized linear regression

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

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

Gradient descent

θ_0 $\qquad \theta_1, \theta_2, \dots, \theta_n$

$\frac{\partial}{\partial\theta_0} J(\theta)$

Repeat {

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

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

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

}

$J(\theta)$

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

$\boxed{\theta_j^2}$

$1 - \alpha\frac{\lambda}{m} < 1$ $\qquad 0.99$ $\qquad \theta_j \times 0.99$

Normal equation

$$X = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \qquad y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix} \in \mathbb{R}^m$$

$m \times (n+1)$

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

$$\theta = \Big(X^T X + \lambda \underbrace{\begin{bmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \\ & & & & 1 \end{bmatrix}}_{(n+1)\times(n+1)} \Big)^{-1} X^T y$$

E.g. $n=2$ $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Non-invertibility (optional/advanced).

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

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

non-invertible / singular

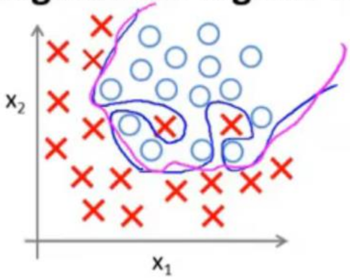
pinv inv

If $\lambda > 0$,

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

4. Regularized logistic regression

Regularized logistic regression.



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

Cost function:

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

$\boxed{\theta_1, \theta_2, \dots, \theta_n}$

Andrew Ng

Gradient descent

Repeat $\{$

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

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

$(j = \cancel{0}, \underbrace{1, 2, 3, \ldots, n}_{\theta_1 \ldots \theta_n})$

$\}$

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

Advanced optimization

$\boxed{\text{fminunc}}$ (@costFunction, ...)

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \begin{array}{l} \text{theta(1)} \\ \text{theta(2)} \\ \\ \text{theta(n+1)} \end{array}$$

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

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

```
    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)];
```

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

$J(\theta)$

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

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

$\vdots$

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