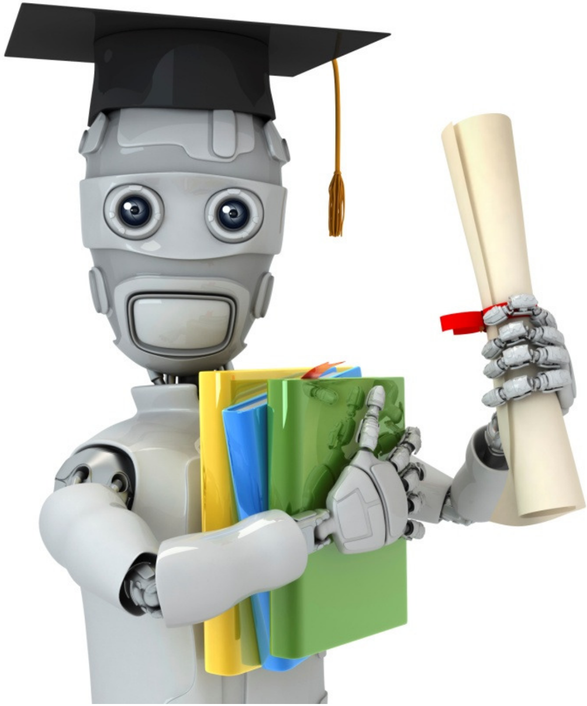


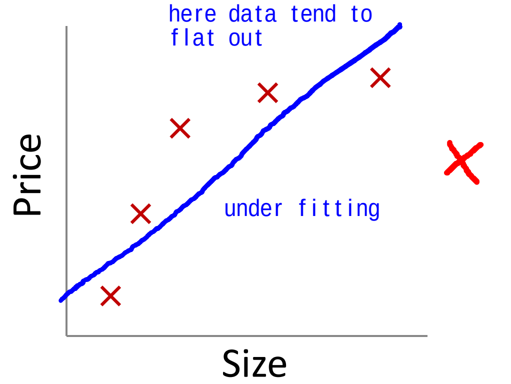
Machine Learning

Regularization

The problem of overfitting

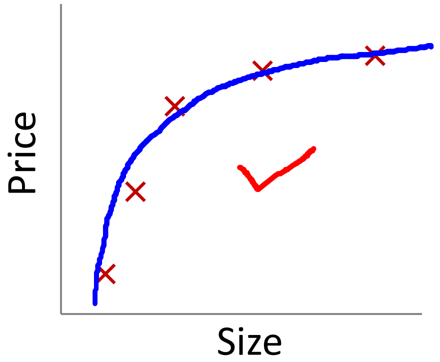
example of overfitting

Example: Linear regression (housing prices)



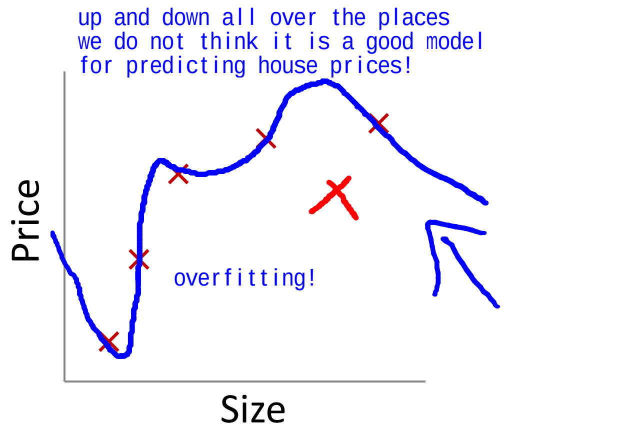
$\rightarrow \theta_0 + \theta_1 x$

"Underfit" "High bias"



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

"Just right"



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

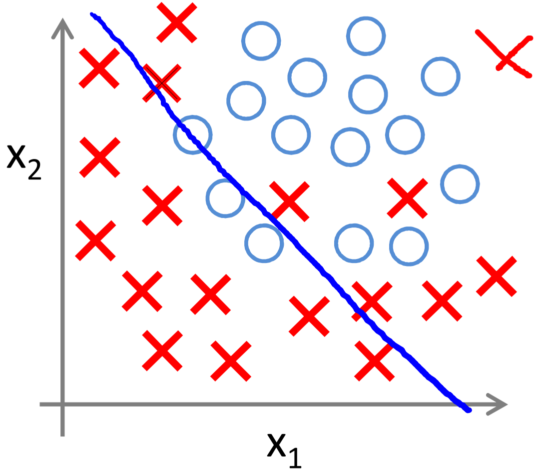
"Overfit" "High variance"

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).

predict!

overfitting examples in logistic regression!

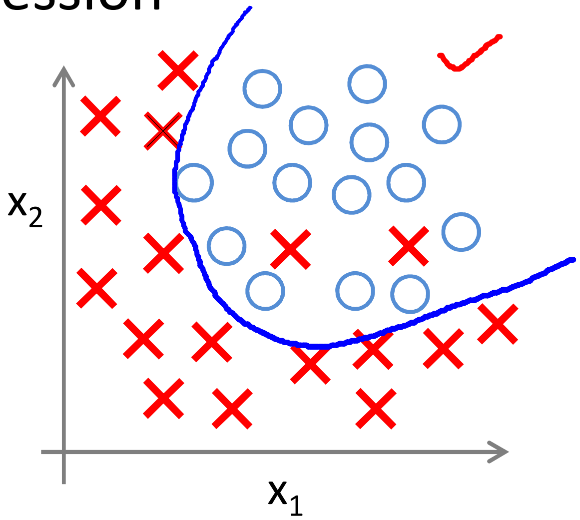
Example: Logistic regression



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

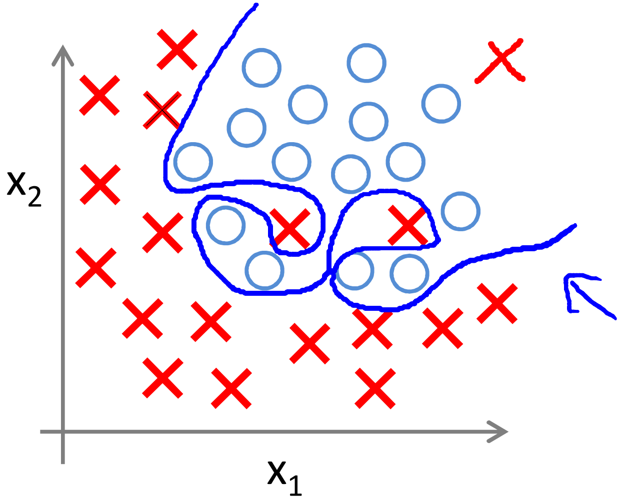
(g = sigmoid function)

"Underfit"



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

this is just right



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

"Overfit"

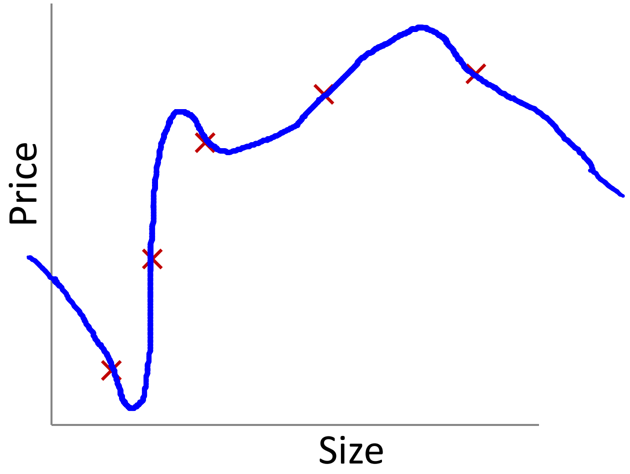
hypothesis has high variance!

Addressing overfitting:

what do we do
when overfitting happens

$x_1 =$ 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}

However, when we have so many features,
it becomes harder to plot the data and
visualize them!

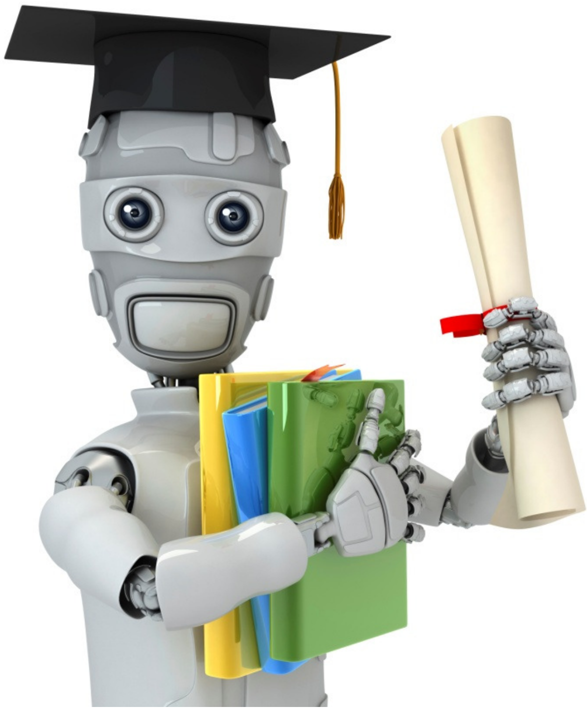


one way to address the overfitting
is to plot the hypothesis function
and look at its shape!

Addressing overfitting: two main options to address overfitting problem

Options:

1. Reduce number of features.
   - Manually select which features to keep.
   - Model selection algorithm (later in course).
2. Regularization. 正则化
   - 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.



Machine Learning

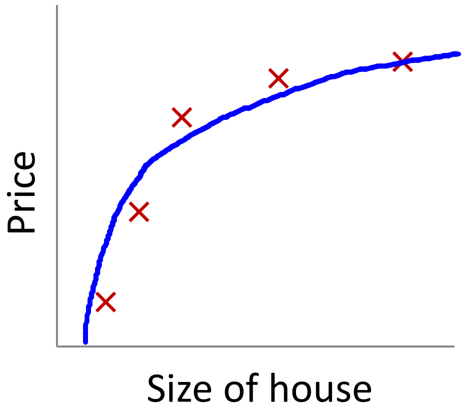
for dealing with overfitting!

Regularization

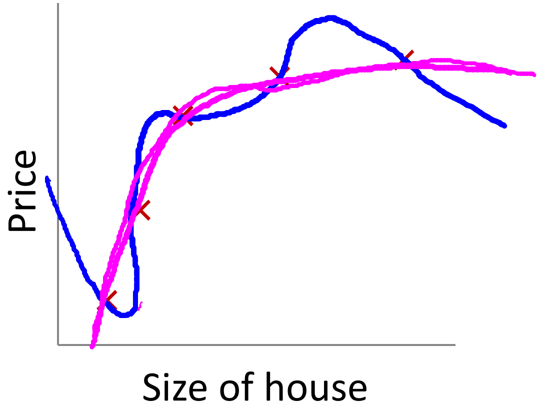
Cost function

intuition of regularization

Intuition



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



a simpler hypothesis
with small theta 3/4

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

Suppose we penalize and make θ_3, θ_4 really small.

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

we minimize this new cost function
so that we can make theta 3,4 very small

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

Andrew Ng

Regularization.

main ideas behind regularization!

Small values for parameters $\boxed{\theta_0, \theta_1, \ldots, \theta_n}$

e.g. we penalize these two parameters to make them very small!

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

- "Simpler" hypothesis
- Less prone to overfitting

an example!

Housing:

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

we do not know which to pick to make small parameters

we add extra regularization term to shrink all the parameters

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

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

by convention we do not regularize theta_0

Andrew Ng

Regularization.

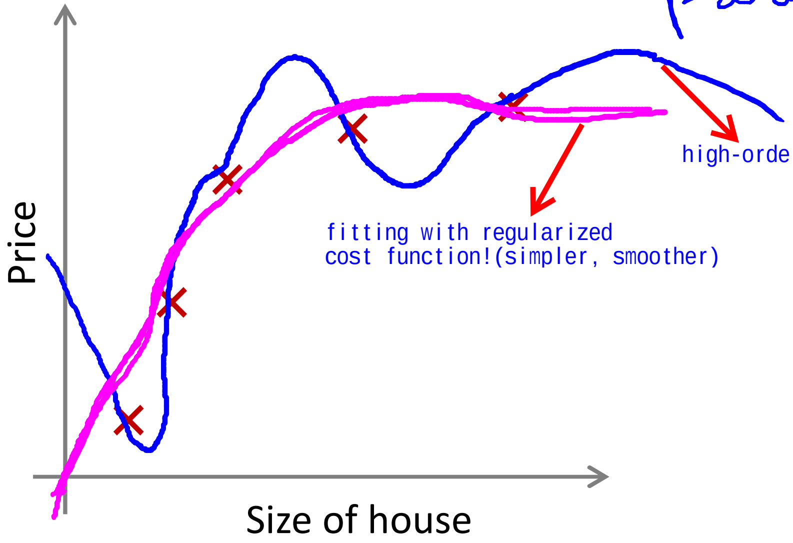
regularized cost function

controls a tradeoff b/c 2 diff goals:
1. fitting the training data well
2. want to keep parameter small, therefore keep the hypothesis simple to avoid overfitting!

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

regularization parameter

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



In regularized linear regression, we choose θ to minimize

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

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

Andrew Ng

In regularized linear regression, we choose θ to minimize

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

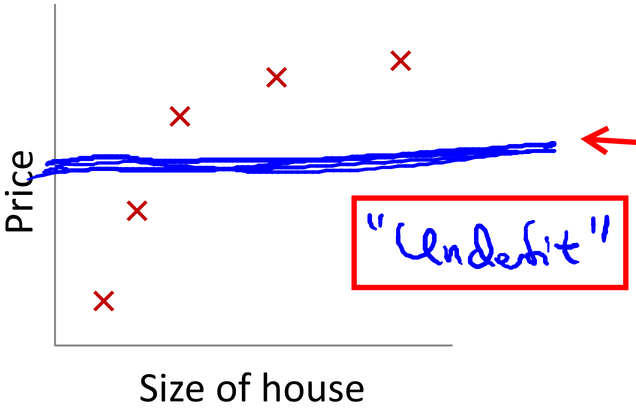
What if λ is set to an extremely large value (perhaps for too large for our problem, say $\lambda = 10^{10}$)?

then we will have

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

$\theta_1 \approx 0, \ \theta_2 \approx 0, \ \theta_3 \approx 0, \ \theta_4 \approx 0$

as a result

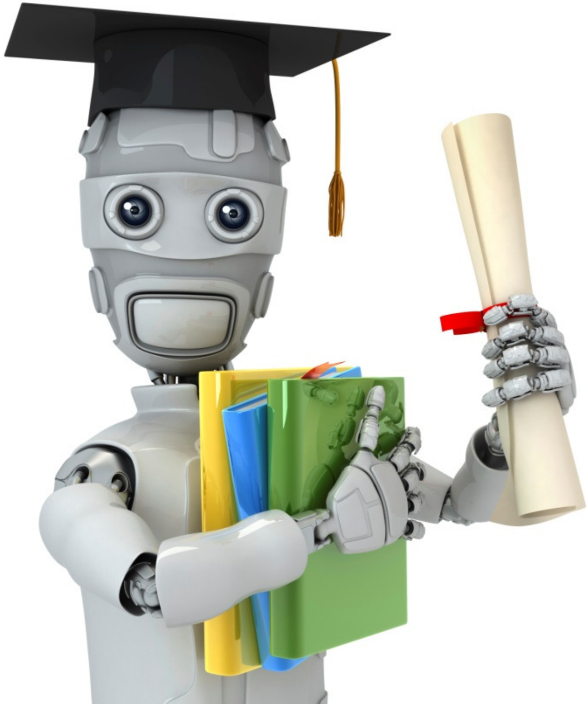


$$\boxed{h_\theta(x) \approx \theta_0}$$

almost flat line!

$h_\theta(x)$

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



Machine Learning

Regularization

Regularized linear regression

two algorithms:
1. gradient descent
2. normal equation

Regularized linear regression

regularization parameter

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

objective!

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

Gradient descent

we do not penalize theta_0 in regularization

$\theta_0 \quad \theta_1, \theta_2, \ldots, \theta_n$

we write theta_0 separately from theta_1,..., since in the regularization term we do not include theta_0

Repeat {

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

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

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

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

}

$\rightarrow J(\theta)$

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

$1 - \alpha \frac{\lambda}{m} < 1$

0.99

$\theta_j \times 0.99$

θ_j

same as the original gradient descent algorithm

Normal equation

m training samples

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

$m \times (n+1)$

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

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

use this to derive this formula

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

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

Non-invertibility (optional/advanced).

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

$$\theta = \underbrace{(X^T X)^{-1}}_{\text{non-invertible / singular}} X^T y$$

pinv inv

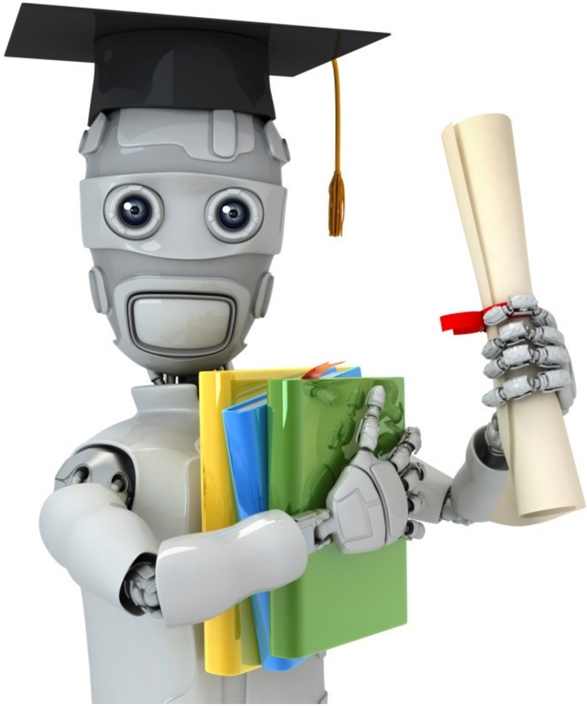
we do not penalize theta_0

Can and has be easily proved!

If $\lambda > 0$,

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

. This can be proved as always invertible! Refer to notes

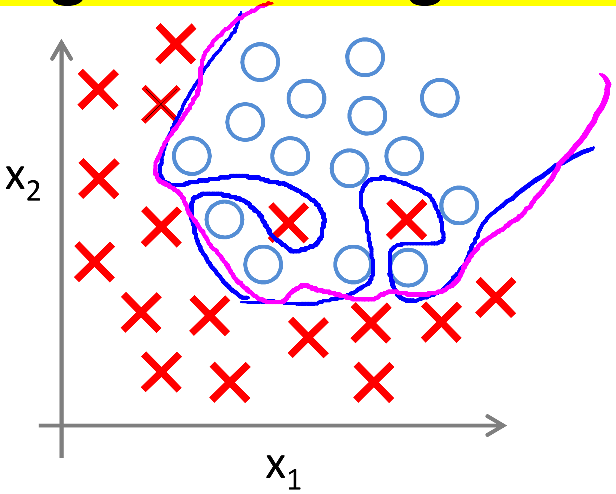


Machine Learning

Regularization

Regularized logistic regression

Regularized logistic regression.



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

Cost function:

add a regularization term!

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

$$+ \boxed{\frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2}$$

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

Gradient descent

even though the algorithm looks identical as in the linear regression case
the hypothesis function is different in the logistic regression case!

Repeat {

update for theta_0

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

new term!

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

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

$\theta_1, \dots, \theta_n$

}

update for theta_1,..n

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

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

Andrew Ng

fminunc(@costFunction...) $\Theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$ theta(1) theta(2) theta(n+1)

Advanced optimization

cost value gradient

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

input

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

need to return the cost function and gradient!

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

regularization term!

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

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

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

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

$J(\theta)$

gradient(3) = [code to compute $\boxed{\frac{\partial}{\partial\theta_2}J(\theta)}$];

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

$\vdots$

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

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