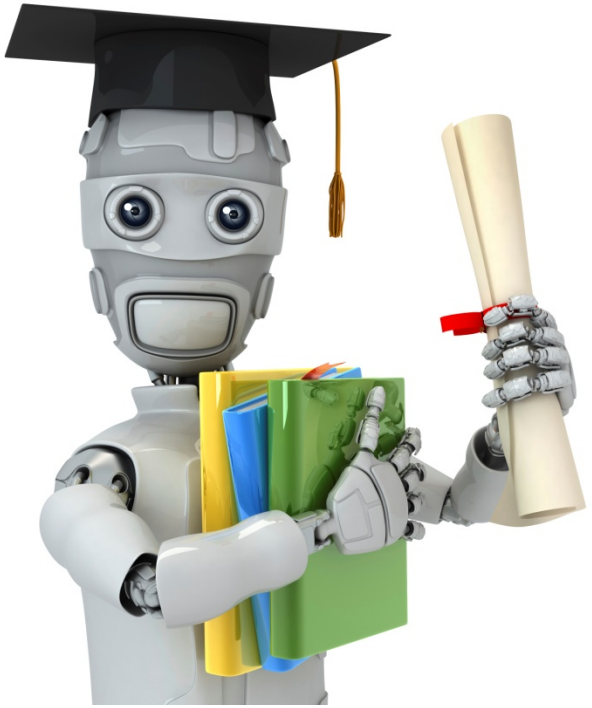
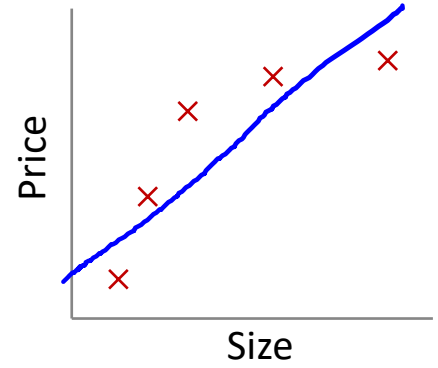


Machine Learning

Regularization

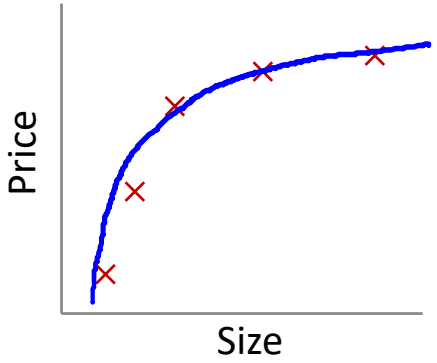
The problem of overfitting

Example: Linear regression (housing prices)



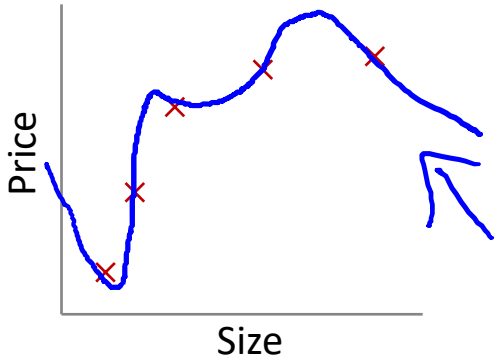
$\rightarrow \theta_0 + \theta_1 x$

"Underfit" "High bias"



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

"Just right"

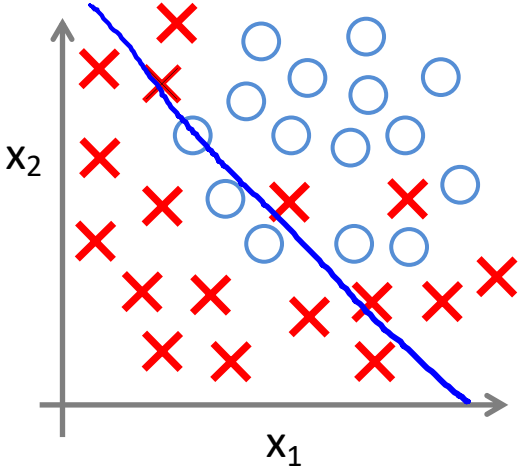


$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

"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).

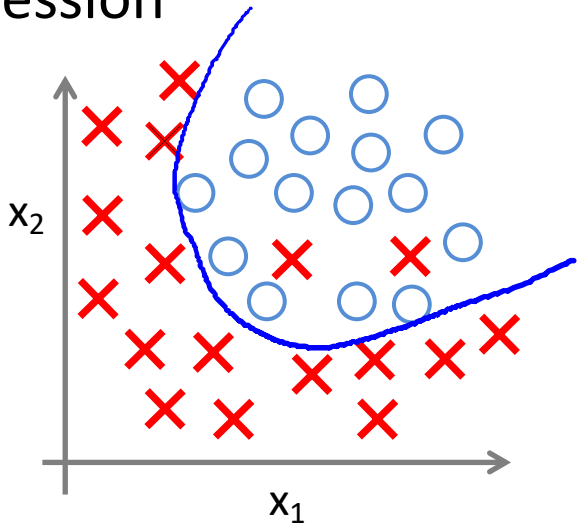
Example: Logistic regression



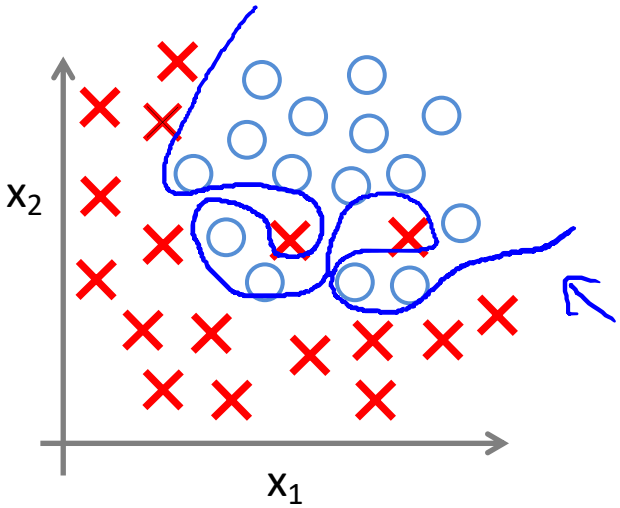
$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

(g = sigmoid function)

"Underfit"



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

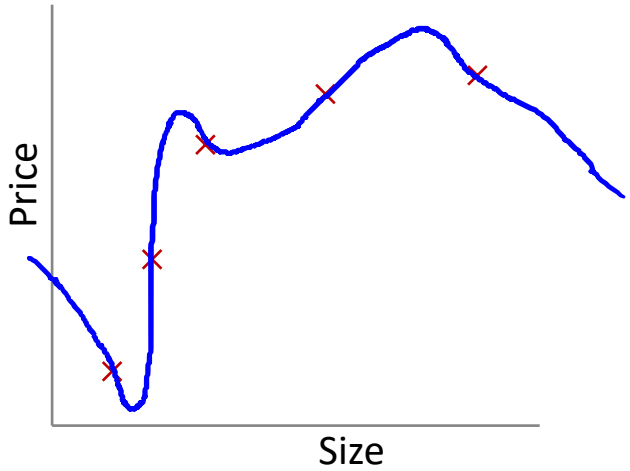


$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$

"Overfit"

Addressing overfitting:

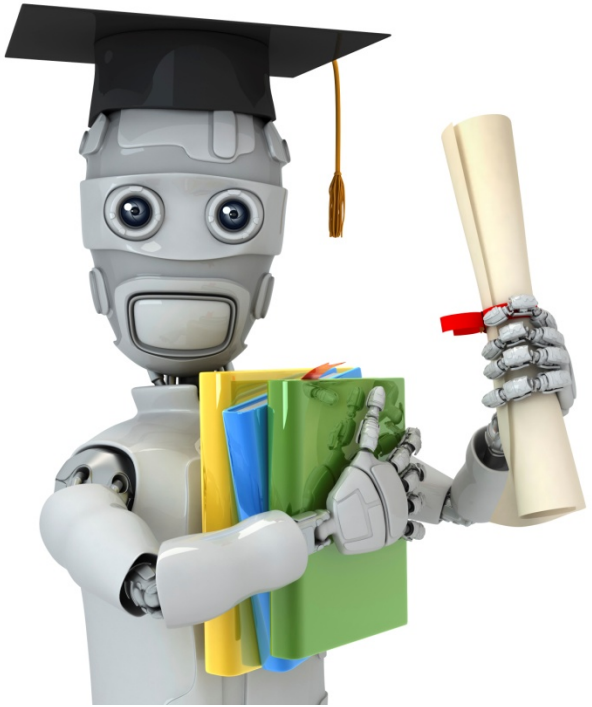
$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size
$\vdots$
x_{100}



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.

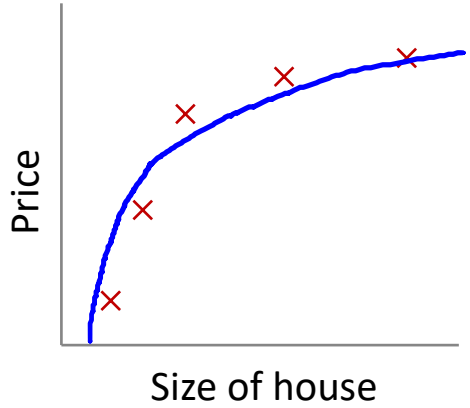


Machine Learning

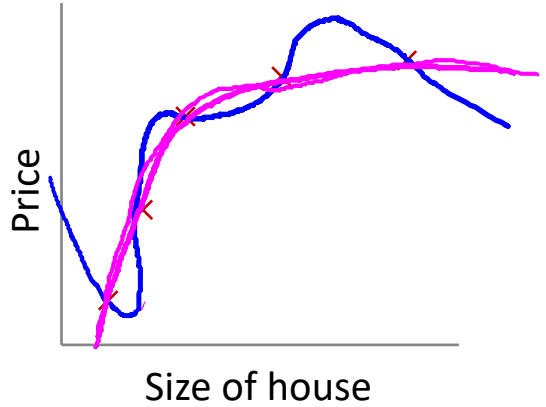
Regularization

Cost function

Intuition



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



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

Suppose we penalize and make θ_3, θ_4 really small.

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

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

Regularization.

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

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

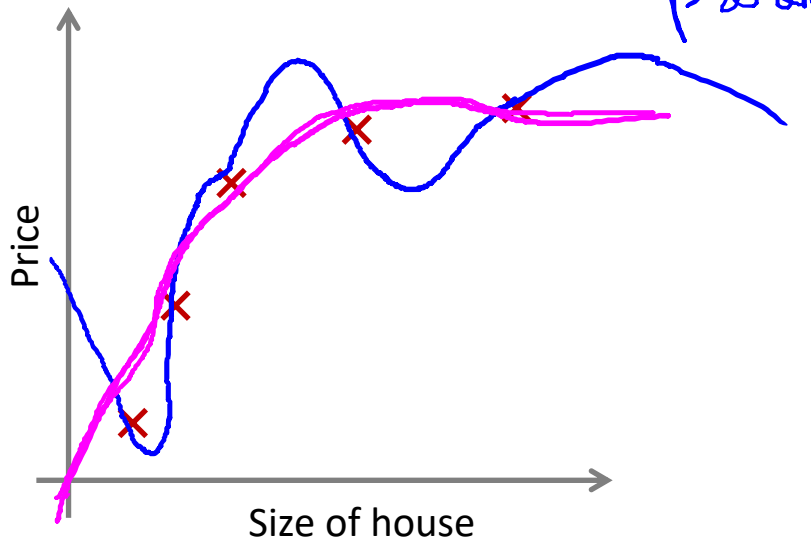
$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} \theta_j^2\right]$$

Regularization.

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

regularization parameter

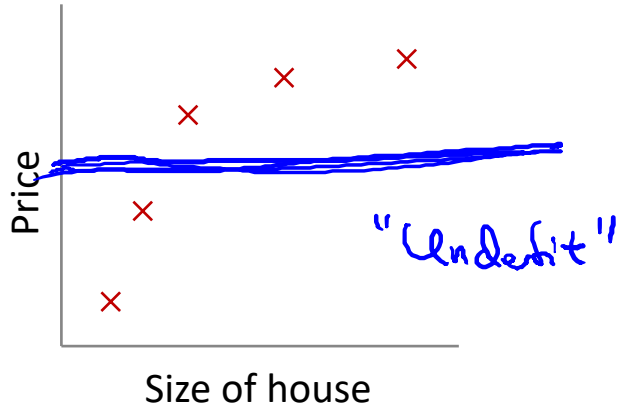
$$\min_\theta J(\theta)$$



In regularized linear regression, we choose θ to minimize

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

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



$h_\theta(x)$

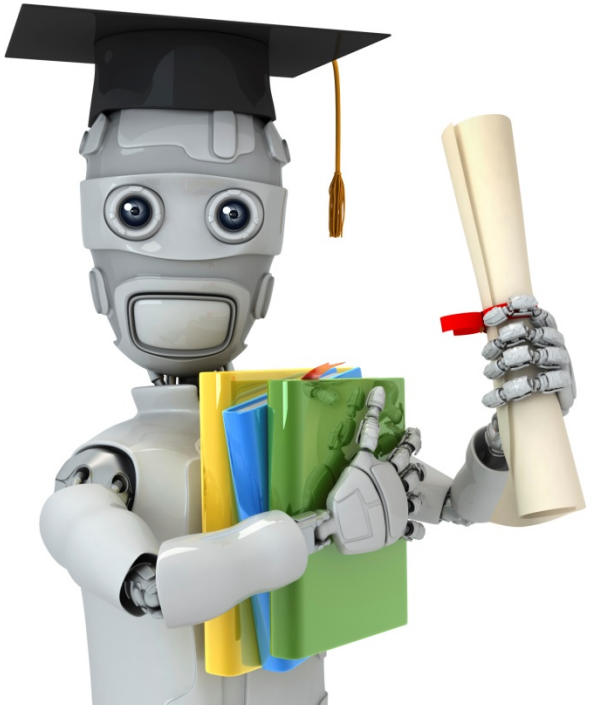
$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

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

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

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

$h_\theta(x) = \theta_0$



Machine Learning

Regularization

Regularized linear regression

Regularized linear regression

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

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

Gradient descent

Repeat $\{$

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

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

$$(j = 1, 2, 3, \ldots, n)$$

$\}$

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

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

0.99

$\theta_j \times 0.99$

θ_j^{I}

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

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

$\rightarrow J(\theta)$

Normal equation

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

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

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

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

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

$(n+1) \times (n+1)$

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)

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

non-invertible / singular

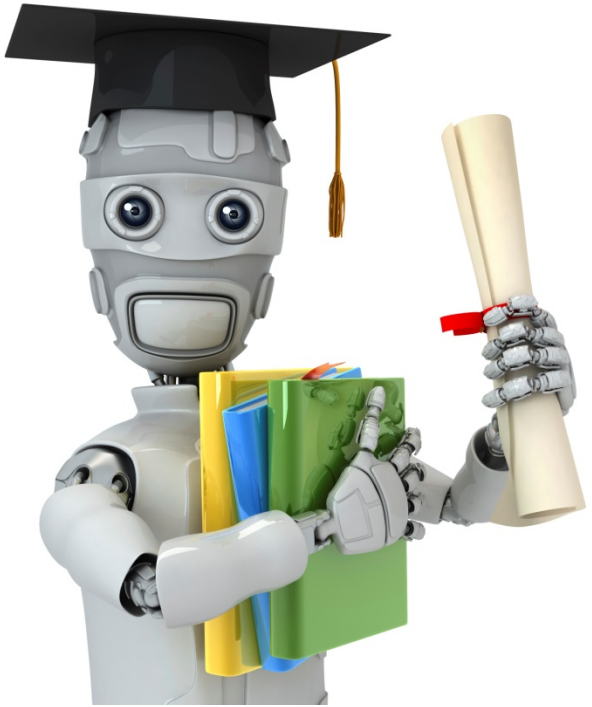
pinv

inv

If $\lambda > 0$,

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

invertible.

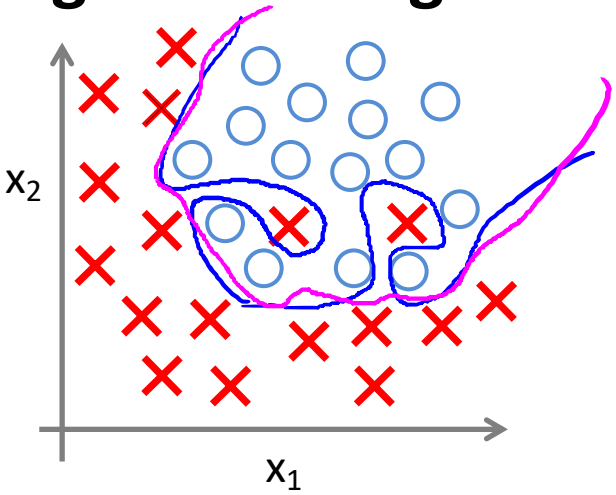


Machine Learning

Regularization

Regularized logistic regression

Regularized logistic regression.



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

Cost function:

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

$\theta_1, \theta_2, \dots, \theta_n$

Gradient descent

Repeat $\{$

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

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

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

$\theta_1 \ldots \theta_n$

$\}$

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

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

Advanced optimization


```
function [jVal, gradient] = costFunction(theta)
    jVal = [code to compute J(θ)];
    gradient(1) = [code to compute ∂/∂θ0 J(θ)];
    gradient(2) = [code to compute ∂/∂θ1 J(θ)];
    gradient(3) = [code to compute ∂/∂θ2 J(θ)];
    :
    gradient(n+1) = [code to compute ∂/∂θn J(θ)];
```

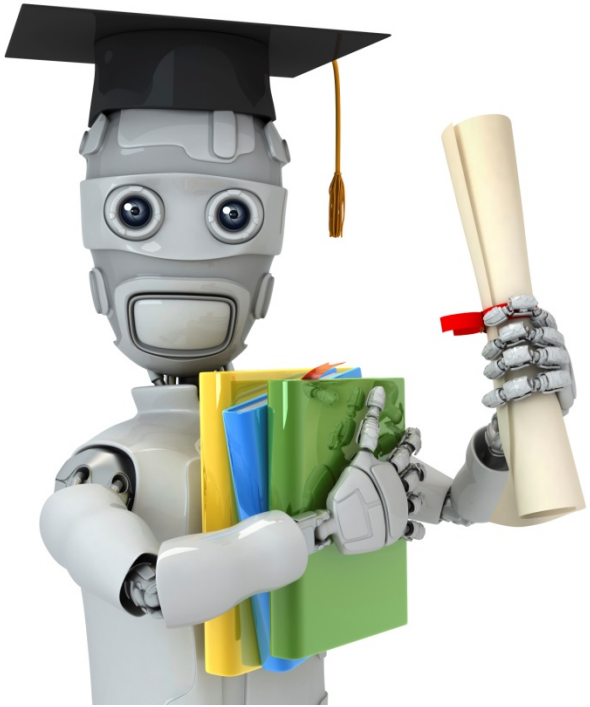
$$J(\theta) = \left[-\frac{1}{m} \sum_{i=1}^{m} y^{(i)} \log\left(h_\theta(x^{(i)}) + (1 - y^{(i)}) \log 1 - h_\theta(x^{(i)})\right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

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

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

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

$J(\theta)$



Machine Learning

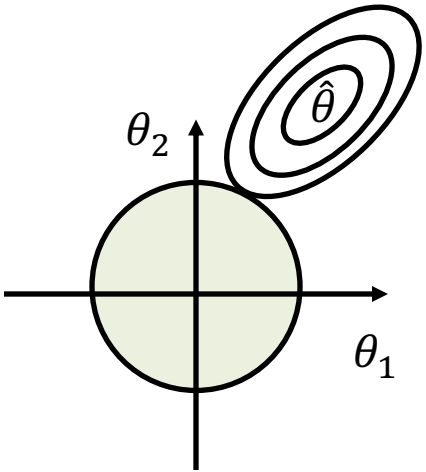
Regularization

Regularizer for sparsity

L2-Norm vs L1-Norm

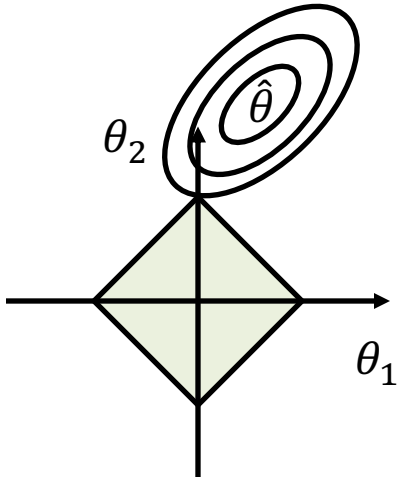
$$\frac{1}{2m}\left[\sum^{\mathrm{m}}(\mathrm{h}_\theta(\mathrm{x})-y)^2+\lambda\sum_{\mathrm{j}=1}^{\mathrm{n}}\theta_{\mathrm{j}}^2\right]$$

$$\theta_1^2+\theta_2^2\leq \mathrm{S}$$



$$\frac{1}{2m}\left[\sum^{\mathrm{m}}(\mathrm{h}_\theta(\mathrm{x})-y)^2+\lambda\sum_{\mathrm{j}=1}^{\mathrm{n}}\left|\theta_{\mathrm{j}}\right|\right]$$

$$\left|\theta_1\right|+\left|\theta_2\right|\leq \mathrm{S}$$



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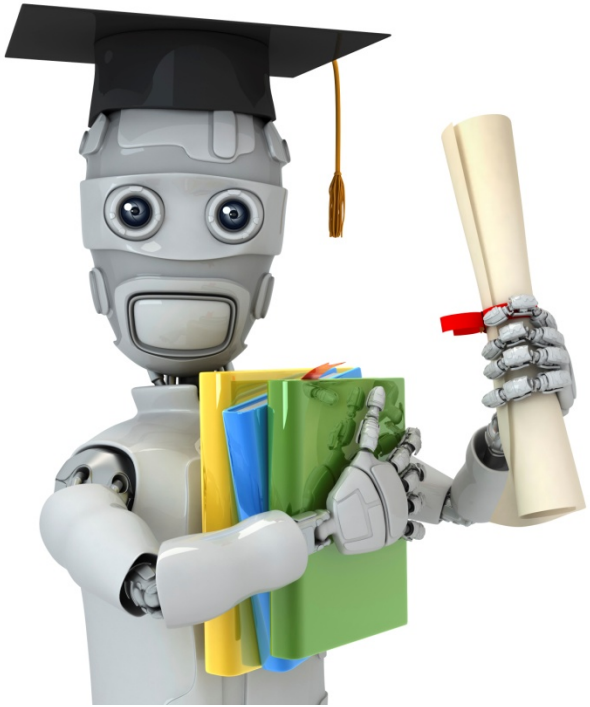


Machine Learning

Validation

Validation

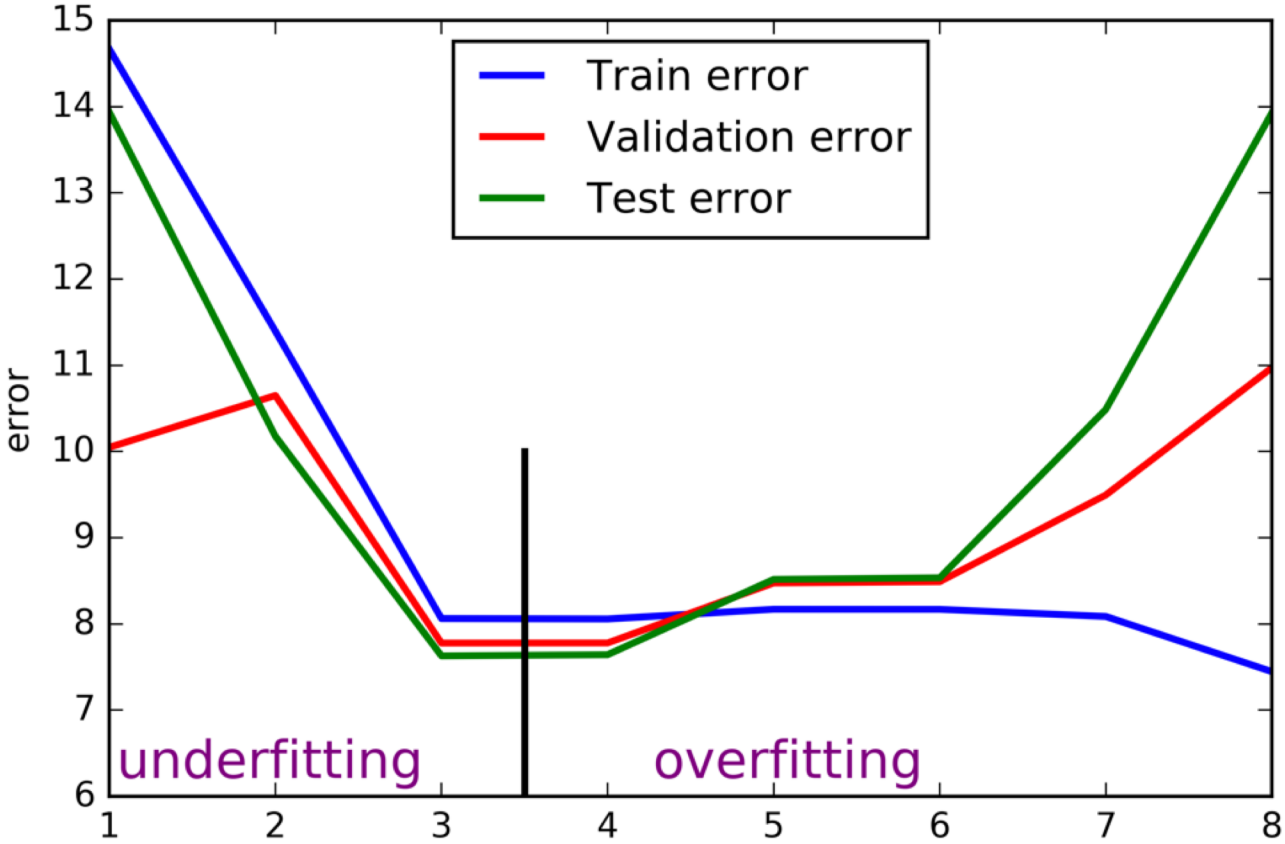
We often divide datasets into two sets:

- training data
- test data (not use in training phase)

How to know the quality of training model with unseen data?

- Extract a small set from training dataset → validation set
- Select the model that provides the small error in both training set and validation set

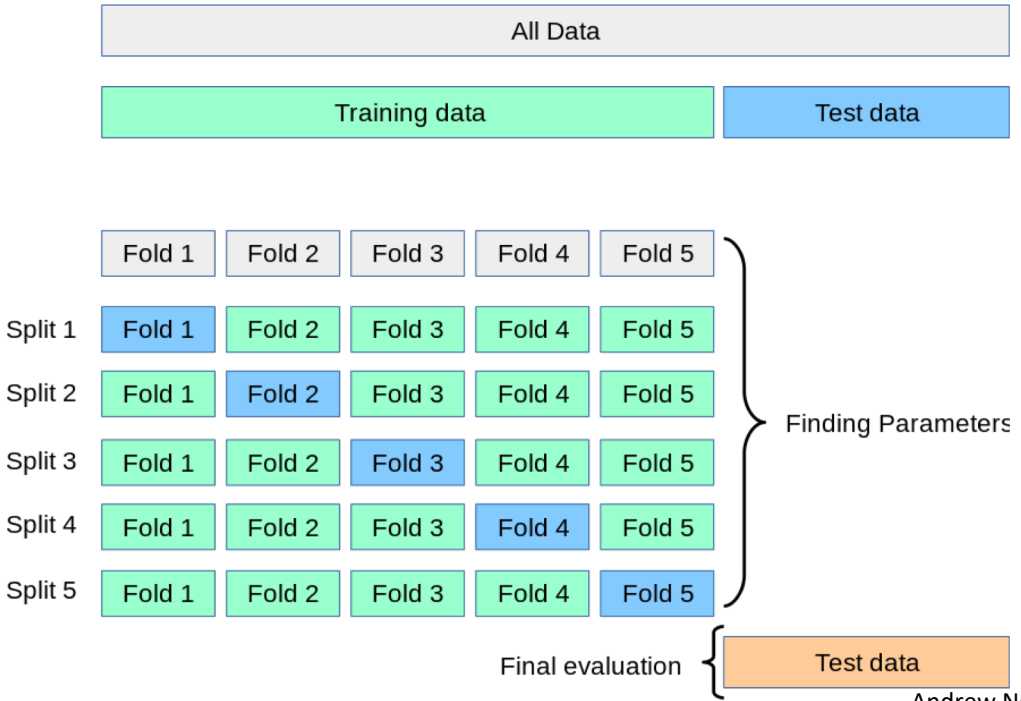
Validation


Train error
Validation error
Test error
error
15
14
13
12
11
10
9
8
7
6
1
2
3
4
5
6
7
8
underfitting
overfitting

Cross-Validation

If the training dataset is very small, taking too much data from it to form validation set will affect the performance → k-fold cross val.

- Split the training set into k sub-sets
- At each run, one of k sub-sets is treated as validation set
- The rest (k-1) sub-sets are treated as training set



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