

Machine Learning

Regularization

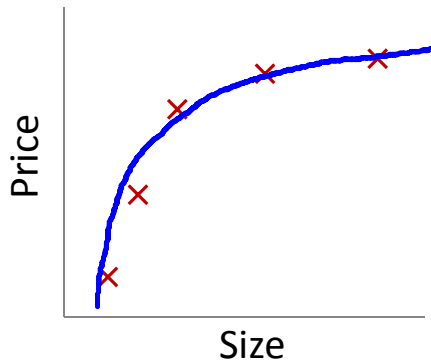
The problem of
overfitting

Example: Linear regression (housing prices)



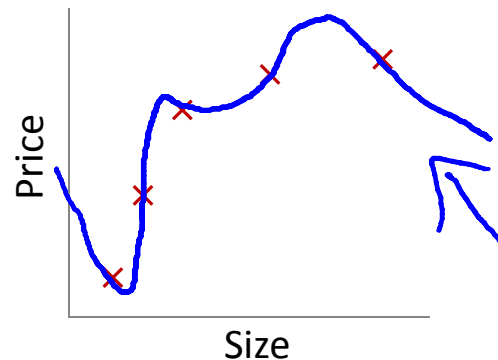
$$\rightarrow \theta_0 + \theta_1 x$$

"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

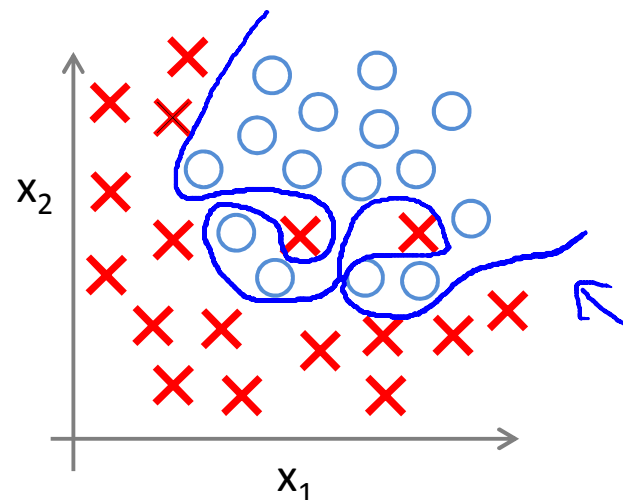


$\rightarrow h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$
 (g = sigmoid function)

"Underfit"



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



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

"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



Size of house

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



Size of house

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

↑
↑

Suppose we penalize and make θ_3, θ_4 really small.

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

$\underline{\theta_3 \approx 0}$
 $\underline{\theta_4 \approx 0}$

Regularization.

Small values for parameters $\theta_0, \theta_1, \dots, \theta_n$

- “Simpler” hypothesis
- Less prone to overfitting

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

Housing:

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

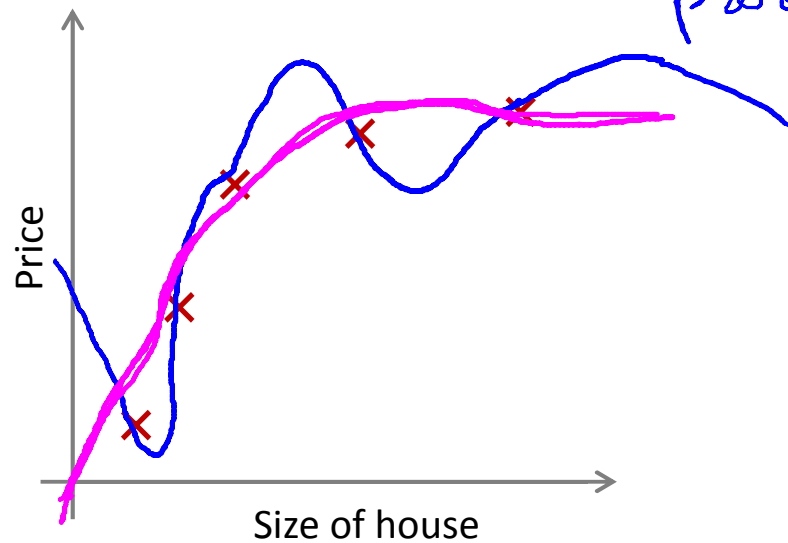
$$J(\theta) = \frac{1}{2m} \left[\sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^n \theta_j^2 \right]$$

~~θ_0~~ $\theta_1, \theta_2, \theta_3, \dots, \theta_{100}$ ~~θ_0~~

Regularization.

$$\rightarrow J(\theta) = \frac{1}{2m} \left[\underbrace{\sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2}_{\text{data fit}} + \underbrace{\lambda \sum_{j=1}^n \theta_j^2}_{\text{regularization parameter}} \right]$$

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



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 far too large for our problem, say $\lambda = 10^{10}$)?

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

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 far too large for our problem, say $\lambda = 10^{10}$)?



$h_{\theta}(x)$

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

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

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

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

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



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

$$\theta_0$$

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

Repeat {

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

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

$$\theta_j := \theta_j - \alpha$$

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

$$+ \frac{\lambda}{m} \theta_j$$

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

}

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

$$\rightarrow J(\theta)$$

$$\theta_j^2$$

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

$$0.99$$

$$\theta_j \times 0.99$$

Normal equation

$$\underline{X} = \begin{bmatrix} (x^{(1)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix} \leftarrow$$

$m \times (n+1)$

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

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

$$\Rightarrow \Theta = \left(X^T X + \lambda \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{(n+1) \times (n+1)} \right)^{-1} X^T y$$

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

$\in \mathbb{R}^n \quad n=2 \quad \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Non-invertibility (optional/advanced).

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

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

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

pinv

inv
 \nearrow

If $\lambda > 0$,

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

$\underbrace{\hspace{10em}}_{\text{invertible .}}$



Machine Learning

Regularization

Regularized
logistic regression

Regularized logistic regression.



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

Handwritten blue arrows point to $\theta_1 x_1$ and $\theta_2 x_1^2$. A handwritten pink arrow points to the $\theta_5 x_1^2 x_2^3$ term.

Cost function:

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

A handwritten pink box encloses the parameters $\theta_1, \theta_2, \dots, \theta_n$.

Gradient descent

Repeat {

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

$$\rightarrow \theta_j := \theta_j - \alpha \left[\underbrace{\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}}_{\substack{(j = \cancel{0}, 1, 2, 3, \dots, n) \\ \theta_1, \dots, \theta_n}} + \frac{1}{n} \theta_j \right] \leftarrow$$

}

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

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

Advanced optimization

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

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

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

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

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

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

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

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

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

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

f_{minunc} (a cost function) $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$ $\theta_0 \leftarrow \text{theta}(1)$
 $\theta_1 \leftarrow \text{theta}(2)$
 $\theta_n \leftarrow \text{theta}(n+1)$

$J(\theta)$

