Machine Learning Study Week 3

Logistic Regression & Regularization



Logistic Regression

Classification

Machine Learning

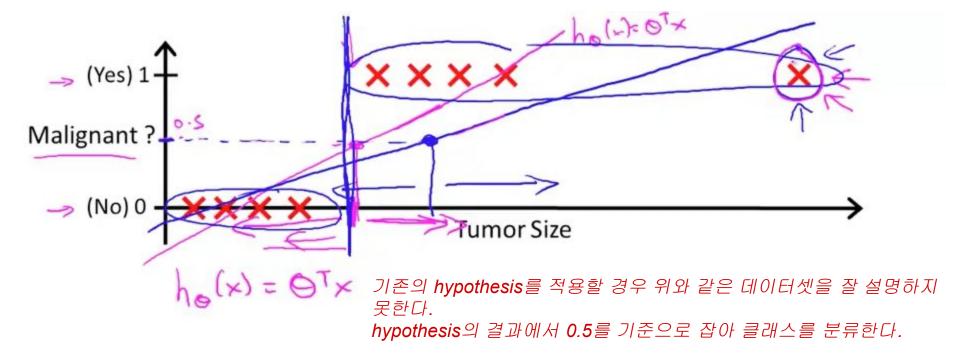
Classification

- → Email: Spam / Not Spam?
- → Online Transactions: Fraudulent (Yes / No)?
- → Tumor: Malignant / Benign?

$$y \in \{0,1\}$$
 0: "Negative Class" (e.g., benign tumor) 1: "Positive Class" (e.g., malignant tumor)

Regression: the output variable takes continuous values.

Classification: the output variable takes class labels.



 \rightarrow Threshold classifier output $h_{\theta}(x)$ at 0.5:

$$\rightarrow$$
 If $h_{\theta}(x) \geq 0.5$, predict "y = 1"

If $h_0(r) < 0.5$ predict "v = 0"

Classification:
$$y = 0$$
 or $\frac{1}{\sqrt{x}}$ $h_{\theta}(x)$ can be > 1 or < 0

Logistic Regression:
$$0 \le h_{\theta}(x) \le 1$$

Classification

linear regression은 결과값이 1 초과, 0 미만일 수도 있다. logistic regression은 hypothesis의 예측범위를 0과 1 사이로 제한한다.



Machine Learning

Logistic Regression

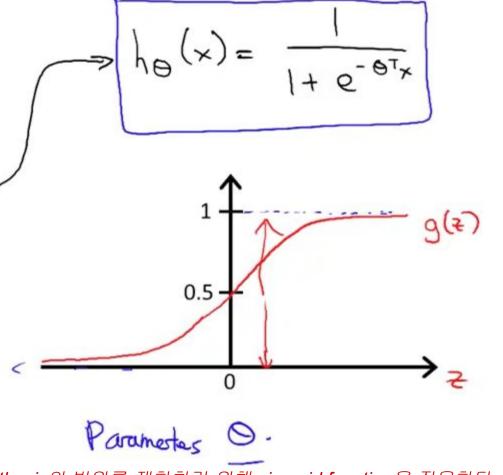
Hypothesis Representation

Logistic Regression Model

Want
$$0 \le h_{\theta}(x) \le 1$$

$$h_{\theta}(x) = 9(\theta^T x)$$

Sigmoid functionLogistic function



hypothesis의 범위를 제한하기 위해 sigmoid function을 적용한다.

Interpretation of Hypothesis Output

$$h_{\theta}(x)$$
 = estimated probability that $y = 1$ on input $x \leftarrow$

Example: If
$$\underline{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \leftarrow \\ \text{tumorSize} \end{bmatrix} \leftarrow h_{\theta}(\underline{x}) = 0.7$$

Tell patient that 70% chance of tumor being malignant

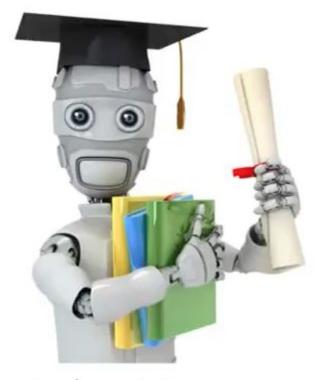
$$h_{\Theta}(x) = P(y=1|x;\Theta)$$

입력 x에 대해 y가 1일 확률을 추정하는 hypothesis.

"probability that y = 1, given x, parameterized by θ''

$$P(\underline{y=0}|x;\theta) + P(\underline{y=1}|x;\theta) = \underline{1}$$

$$P(\underline{y=0}|x;\theta) = 1 - P(\underline{y=1}|x;\theta)$$



Machine Learning

Logistic Regression

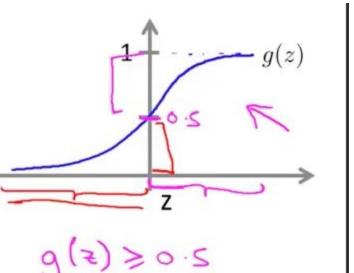
Decision boundary

Logistic regression

$$\rightarrow h_{\theta}(x) = g(\theta^T x) = P(y=1|x:\theta)$$

$$g(z) = \frac{1}{1+e^{-z}}$$
Suppose predict $y = 1$ if $y = 1$ if $y = 1$.

0.5 미만이면 y=0으로 예상한다.



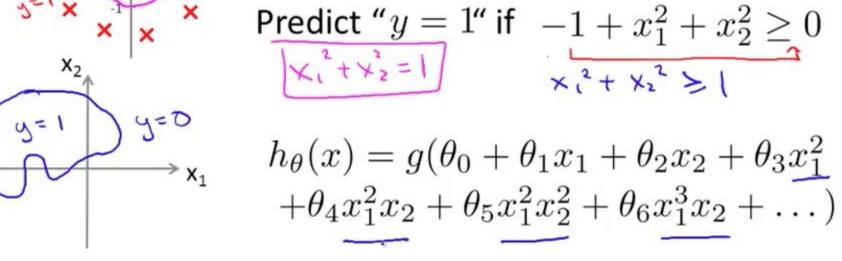
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ho(x) = 9 (otx) >0.5

0= 1 -3 E **Decision Boundary** $h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$ Decision boundary 4=01 Predict "y = 1" if $-3 + x_1 + x_2 \ge 0$ OTX X1+X2 >3 logistic regression에서 hypothesis의 결과가 1이 되는 경계가 존재한다.

Non-linear decision boundaries

$$\begin{array}{c} \mathbf{x} \\ \mathbf{$$





Logistic Regression

Cost function

Machine Learning

Training set:
$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})\}$$

How to choose parameters θ ?

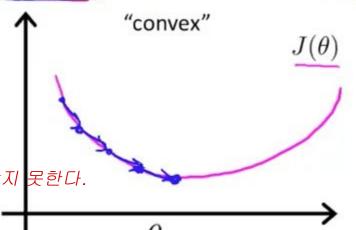


>> Linear regression:

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

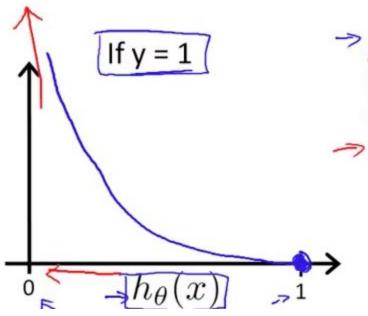
$$\operatorname{Cost}(h_{\theta}(x^{\bullet}), y^{\bullet}) = \left[\frac{1}{2} \left(h_{\theta}(x^{\bullet}) - y^{\bullet}\right)^{2} \right] \leftarrow$$





Logistic regression cost function

$$Cost(\underline{h_{\theta}(x)}, y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$



Captures intuition that if $h_{\theta}(x) = 0$, (predict $P(y = 1|x; \theta) = 0$), but y = 1, we'll penalize learning algorithm by a very large cost.

Logistic regression cost function

$$\operatorname{Cost}(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$

$$|f y = 0|$$



Machine Learning

Logistic Regression

Simplified cost function and gradient descent

Logistic regression cost function

$$\rightarrow J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \underbrace{\text{Cost}(h_{\theta}(x^{(i)}), y^{(i)})}_{}$$

$$\operatorname{Cost}(h_{\theta}(x), y) = \begin{cases} -\log(h_{\theta}(x)) & \text{if } y = 1 \\ -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases}$$

Note: y = 0 or 1 always

Logistic regression cost function

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

To fit parameters θ :

$$\min_{\theta} J(\theta)$$
 Gret Θ

To make a prediction given new x:

Output
$$h_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$
 $p(y=1 \mid x; \Theta)$

Gradient Descent

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

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

Repeat {
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$
 { (simultaneously update all θ_j) }
$$\frac{\partial}{\partial \phi} J(\phi) = \frac{1}{M} \sum_{i=1}^{\infty} \left(h_{\phi}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)} \right) \times_j^{(i)}$$

J_of_theta를 최저로 만드는 theta를 찾기 위해 gradient를 계산한다.

Gradient Descent

Algorithm looks identical to linear regression!



Machine Learning

Logistic Regression

Advanced optimization

Optimization algorithm

Given θ , we have code that can compute

$$\begin{array}{c|c} -J(\theta) & \longleftarrow \\ -\frac{\partial}{\partial \theta_j}J(\theta) & \longleftarrow \end{array} \quad \text{(for } j=0,1,\ldots,n \text{)}$$

Optimization algorithms:

- Gradient descent
 - Conjugate gradient
 - BFGS
 - L-BFGS

cost function을 최저로 만드는 theta를 찾는 여러 가지 알고리즘이 존재한다.

Advantages:

- No need to manually pick α
- Often faster than gradient descent.

Disadvantages:

More complex

Example: θ_1 θ_2 θ_3 θ_4 θ_5 θ_5 θ_7 θ

$$\Rightarrow \theta = \begin{bmatrix} \theta_2 \end{bmatrix} \quad \underbrace{\theta_1 = 5, \theta_2 = 5}_{0.25}.$$

$$\Rightarrow J(\theta) = (\theta_1 - 5)^2 + (\theta_2 - 5)^2$$

$$\xrightarrow{\partial} J(\theta) = 2(\theta_1 - 5)^2$$

$$\frac{\partial}{\partial \theta_1} J(\theta) = 2(\theta_1 - 5)$$

$$\frac{\partial}{\partial \theta_2} J(\theta) = 2(\theta_2 - 5)$$

options = optimset('GradObj', 'on', 'MaxIter', '100');

[optTheta, functionVal, exitFlag] ...

function [jVal, gradient] = costFunction(theta) $jVal = (theta(1)-5)^2 + ...$ $(theta(2)-5)^2;$ gradient = zeros(2,1);

gradient(1) = 2*(theta(1)-5);gradient(2) = 2*(theta(2)-5);

= fminunc(@costFunction, initialTheta, options); cost function을 정의하고, 초기값과 함께 전달하면 라이브러리 함수로 optimized theta를 찾아준다.

theta =
$$\begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{cases} \frac{\theta_0}{\theta_1} \\ \frac{\theta_1}{\theta_1} \end{cases}$$
 theta(1)

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

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

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

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



Machine Learning

Logistic Regression

Multi-class classification: One-vs-all

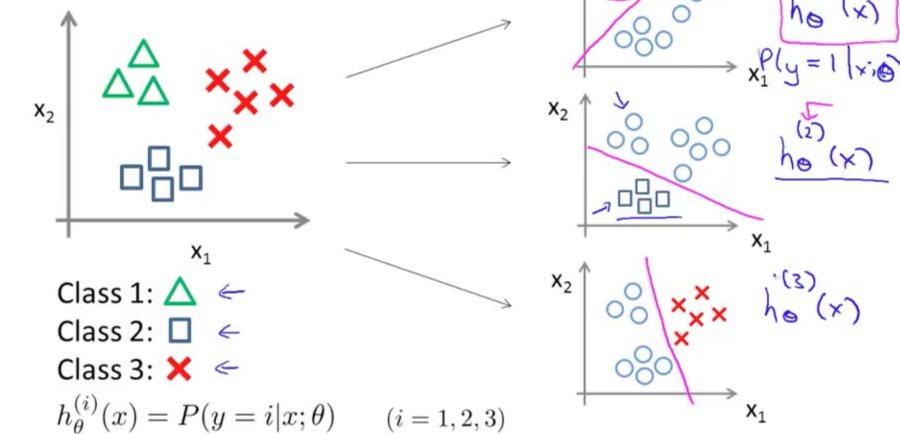
Multiclass classification

Email foldering/tagging: Work, Friends, Family, Hobby

Medical diagrams: Not ill, Cold, Flu

Weather: Sunny, Cloudy, Rain, Snow

One-vs-all (one-vs-rest):



One-vs-all

Train a logistic regression classifier $h_{\theta}^{(i)}(x)$ for each class \underline{i} to predict the probability that $\underline{y}=\underline{i}$.

On a new input \underline{x} , to make a prediction, pick the class i that maximizes

$$\max_{\underline{i}} h_{\theta}^{(i)}(x)$$

각 class에 대해서 one-vs-all로 확률을 구하고, 그 중 가장 높은 hypothesis를 선택한다.

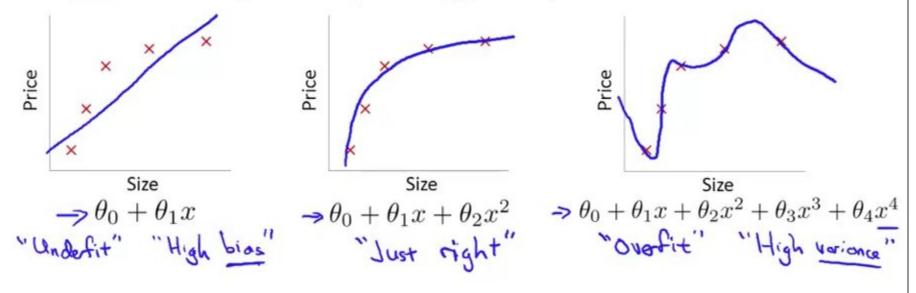


Machine Learning

Regularization

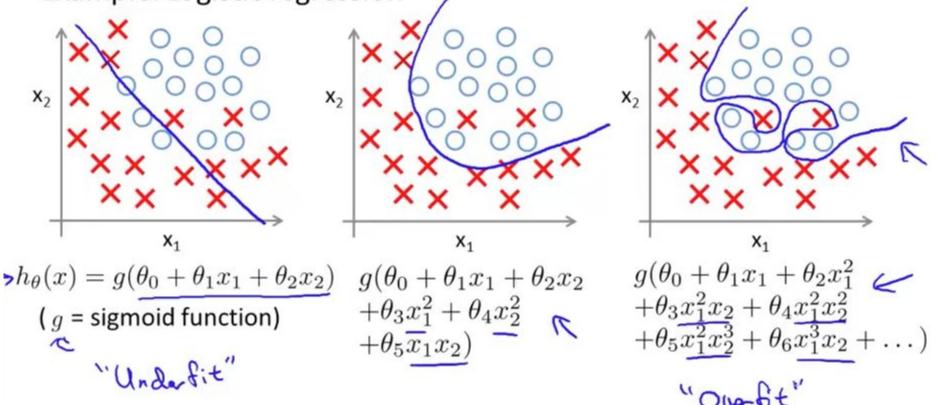
The problem of overfitting

Example: Linear regression (housing prices)



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



Addressing overfitting:

Options:

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

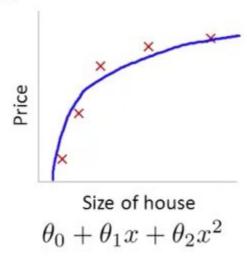


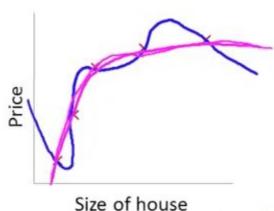
Regularization

Cost function

Machine Learning

Intuition





 $\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^3 + \theta_5 x^3 +$

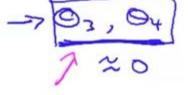
Suppose we penalize and make
$$\theta_3$$
, θ_4 really small.

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

Regularization.

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

- "Simpler" hypothesis
- Less prone to overfitting <



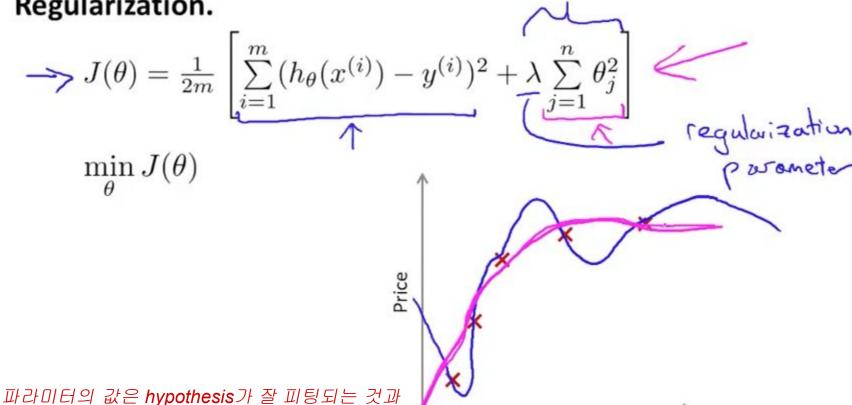
Housing:

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

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



오버피팅을 shrink 시키는 것 사이의 trade off이다.

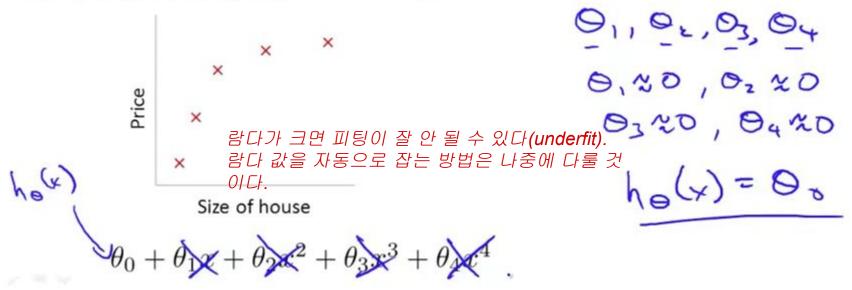


Size of house

In regularized linear regression, we choose θ to minimize

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

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





Machine Learning

Regularization

Regularized linear regression

Gradient descent

Repeat {

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

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

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

$$-\frac{\sigma_j}{\int}$$

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m})$$

$$\bigcirc$$
, \bigcirc , \bigcirc , \bigcirc ,

$$x_0^{(i)}$$
 $\frac{3}{2}$ $\sqrt{2}$ (0)

$$\underbrace{\frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) x_{j}^{(i)}}_{(j = \mathbf{X}, 1, 2, 3, \dots, n)} + \underbrace{\frac{\lambda}{m}}_{m} \mathbf{S}$$

줄어들고, Gradient descent는 동일하게 유지된다.

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



Normal equation

cost function을 최소로 만드는 theta를 방정식으로 푸는 방법

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

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

$$\Rightarrow 0 = (X^T \times + \lambda) \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$\Rightarrow \sum_{\theta = 0}^{\infty} (x^{(1)})^T$$

$$\Rightarrow \sum_{\theta = 0}^{\infty} J(\theta) = \sum_{\theta = 0}^{\infty} (x^{(1)})^T$$

$$\Rightarrow \sum_{\theta = 0}^{\infty} J(\theta) = \sum_{\theta = 0}^{\infty} (x^{(1)})^T$$

$$\Rightarrow \sum_{\theta = 0}^{\infty} J(\theta) = \sum_{\theta = 0$$

Non-invertibility (optional/advanced).

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

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

If
$$\lambda > 0$$

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

non-invertible 했던 문제가 regularization으로 invertible 해졌다.

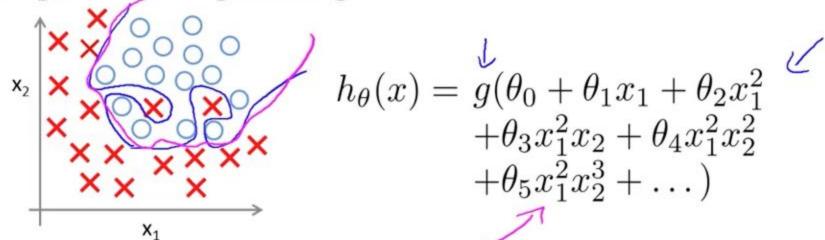


Machine Learning

Regularization

Regularized logistic regression

Regularized logistic regression.



Cost function:

logistic regression에도 적용 가능하다. feature가 많은 경우에도 regularization이 효과가 있다.

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

$$+ \frac{\lambda}{2m} \sum_{i=1}^{n} \mathcal{O}_{i}^{2} \qquad \boxed{\mathcal{O}_{i}, \mathcal{O}_{i}, \dots, \mathcal{O}_{n}}$$

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Gradient descent

Repeat {

$$\theta_{0} := \theta_{0} - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x^{(i)}) - y^{(i)}) x_{0}^{(i)}$$

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

$$\left(\underbrace{j = \mathbf{x}, 1, 2, 3, \dots, n}_{\mathbf{x}_{1}, \dots, \mathbf{x}_{n}} \right)$$

Gradient descent에서 linear regression과 같은 외형을 보이지만 hypothesis가 다르다.

Advanced optimization

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

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

$$\longrightarrow$$
 gradient(1) = [code to compute $\left[\frac{\partial}{\partial \theta_0}J(\theta)\right]$; $\frac{1}{m}\sum_{i=1}^{m}(h_{\theta}(x^{(i)})-y^{(i)})x_0^{(i)}$ \longleftarrow

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

$$: \left(rac{1}{m}\sum_{i=l}^{m}(h_{ heta}(x^{(i)})-y^{(i)})x_{2}^{(i)}
ight)+rac{\lambda}{m} heta_{2}$$
 regularization으로 적용한 gradient를 advanced optimization에도 적용 가능하

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