Machine Learning Formulae

Notations

m = Number of training examples.

n = Number of features.

$x^{(i)}$ = The features of the i_{th} training example, which is an $n+1$ vector.

$y^{(i)}$ = The Target value of the i_{th} training example, which is a number.

$(x^{(i)}, y^{(i)})$ = The i_{th} training example.

$x_j^{(i)}$ = The j_{th} feature of the i_{th} training example, which is a number.

α = Learning rate

Multivariate Linear Regression

Hypothesis

$h_x(\theta) = \sum_{i=0}^{n} \theta_i x_i$ x_0 is always equal to 1.

Cost Function

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

Gradient Desecnt

`Repeat{`

$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$

$(j = 0, 1, 2, \ldots, n)$, α stands for learning rate.

`}`

Calculate the $\frac{\partial}{\partial \theta_j} J(\theta)$, which means the partial derivative respect to θ_j:

`Repeat{`

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

`}`

Feature Scaling

Replace every x with:

$\frac{x-\mu}{s}$

μ stands for the average of x's, and s stands for the standard deviation of x's.

Normal Equation

Define the feature vector of the i_{th} training example:

$$x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \dots \\ x_n^{(i)} \end{bmatrix}$$ $x^{(i)}$ is an $n+1$ vector.

Define ***design matrix*** X:

$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \dots \\ (x^{(m)})^T \end{bmatrix}$$ X is an $m \times (n+1)$ matrix.

Define the target value vector:

$$y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \dots \\ y^{(m)} \end{bmatrix}$$ y is an $m \times (n+1)$ vector.

Then, we can calculate θ:

$\theta = (X^T X)^{-1} X^T y$ θ Is an $n+1$ vector.

Logistic Regression

Hypothesis

Define:

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{bmatrix} \quad x = \begin{bmatrix} x_0 \\ x_1 \\ \dots \\ x_n \end{bmatrix}$$

Hypothesis:

$h_\theta(x) = g(\theta^T x)$

$g(z) = \frac{1}{1+e^{-z}}$ (sigmoid/logistic function)

which means:

$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}} \in (0,1)$

Cost Function

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

$$Cost(h_\theta(x^{(i)}), y^{(i)}) = \begin{cases} -log(1-h_\theta(x)), & y=0 \\ -log(h_\theta(x)), & y=1 \end{cases} \iff Cost(h_\theta(x^{(i)}), y^{(i)}) = -ylog(h_\theta(x)) - (1-y)log(1-h_\theta(x))$$

Gradient Descent

`Repeat{`

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

`}`

Multiclass Classification

Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i to predict the probability that $y=i$. On a new input x, to make a prediction, pick the class i that maximizes $h_\theta^{(i)}(x)$.

Regularized Linear Regression

Cost Function

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

Gradient Descent

`Repeat{`

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

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

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

`}`

Normal Equation

$$\theta = (X^TX + \lambda\begin{bmatrix} 0 & 0 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 0 & 1 & \ldots & 0 \\ \ldots \\ 0 & 0 & 0 & 0 & \ldots & 1 \end{bmatrix})^{-1}X^Ty$$

Regularized Logistic Regression

Cost Function

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

Gradient Desecnt

`Repeat{`

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

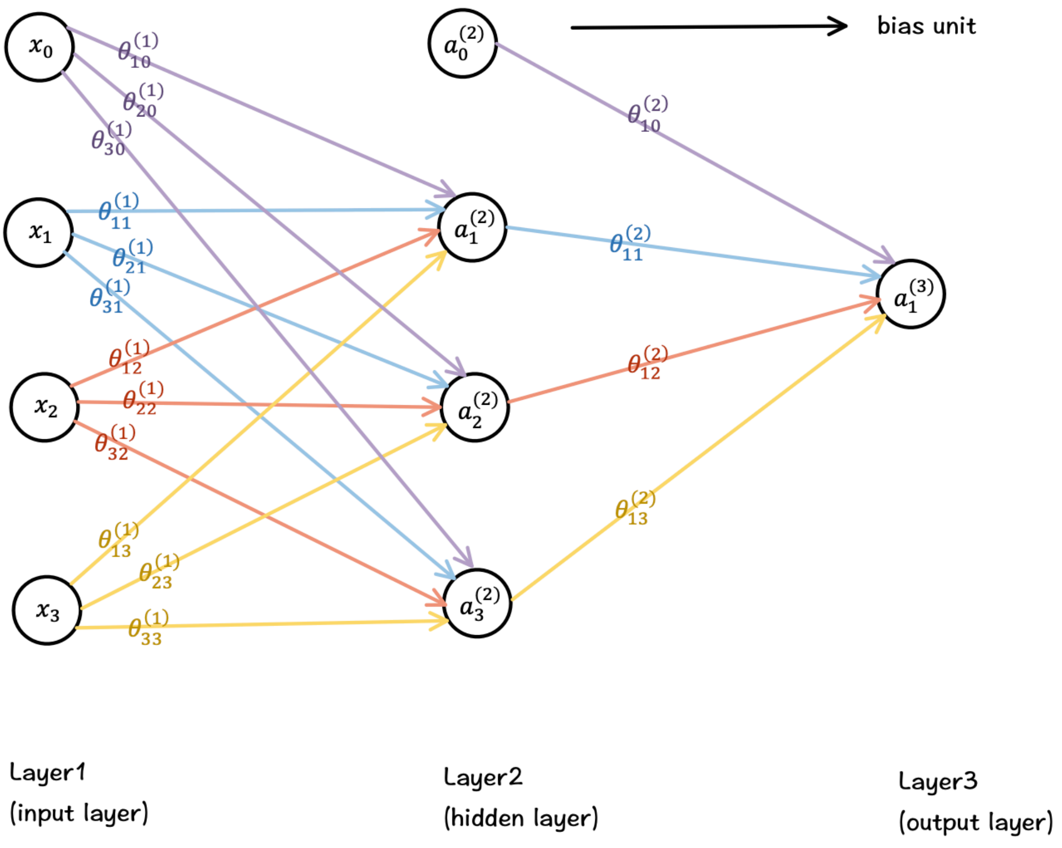
$\theta_j := \theta_j - \alpha[\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} + \frac{\lambda}{m}\theta_j]$

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

`}`

Neural Network

Architecture



$a_i^{(j)}$ = activation of unit i in layer j

$\theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$

E.g.

X= $\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}$ $\theta^{(1)} = \begin{bmatrix} \theta_{10}^{(1)} & \theta_{11}^{(1)} & \theta_{12}^{(1)} & \theta_{13}^{(1)} \\ \theta_{20}^{(1)} & \theta_{21}^{(1)} & \theta_{22}^{(1)} & \theta_{23}^{(1)} \\ \theta_{30}^{(1)} & \theta_{31}^{(1)} & \theta_{32}^{(1)} & \theta_{33}^{(1)} \end{bmatrix} \in R^{3\times 4}$

$a_1^{(2)} = g(\theta_{10}^{(1)}x_0 + \theta_{11}^{(1)}x_1 + \theta_{12}^{(1)}x_2 + \theta_{13}^{(1)}x_3)$ Define: $z_1^{(2)} = \theta_{10}^{(1)}x_0 + \theta_{11}^{(1)}x_1 + \theta_{12}^{(1)}x_2 + \theta_{13}^{(1)}x_3$

$a_2^{(2)} = g(\theta_{20}^{(1)}x_0 + \theta_{21}^{(1)}x_1 + \theta_{22}^{(1)}x_2 + \theta_{23}^{(1)}x_3)$ Define: $z_2^{(2)} = \theta_{20}^{(1)}x_0 + \theta_{21}^{(1)}x_1 + \theta_{22}^{(1)}x_2 + \theta_{23}^{(1)}x_3$

$a_3^{(2)} = g(\theta_{30}^{(1)}x_0 + \theta_{31}^{(1)}x_1 + \theta_{32}^{(1)}x_2 + \theta_{33}^{(1)}x_3)$ Define: $z_3^{(2)} = \theta_{30}^{(1)}x_0 + \theta_{31}^{(1)}x_1 + \theta_{32}^{(1)}x_2 + \theta_{33}^{(1)}x_3$

$\Longleftrightarrow a^{(2)} = g(\theta^{(1)}X) \Longleftrightarrow a^{(2)} = g(z^{(2)})$

Cost Function

L = total number of layers in network

S_l = number of units(not counting bias unit) in lay l.

$h_\theta(x) \in R^K$ (which means there are K units in the output layer)

$(h_\theta(x))_i$ = i^{th} output

$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} log(h_\theta(x^{(i)}))_k + (1-y_k^{(i)})log(1-(h_\theta(x^{(i)}))_k)] + \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{S_l}\sum_{j=1}^{S_{l+1}}(\theta_{ji}^{(l)})^2$

Back Propagation

Intuition: $\delta_j^{(l)}$ = error of node j in layer l

Suppose $L=4$, that is, there are 4 layers in the network in total:

For each output unit($l=4$):

$\delta_j^{(4)} = a_j^{(4)} - y_j$

Vectorization: $\delta^{(4)} = a^{(4)} - y$

For other layers:

$\delta^{(3)} = (\theta^{(3)})^T\delta^{(4)}.*g^{'}(z^{(3)}) = a^{(3)}.*(1-a^{(3)})$

$\delta^{(2)} = (\theta^{(2)})^T\delta^{(3)}.*g^{'}(z^{(2)}) = a^{(2)}.*(1-a^{(2)})$

...

Algorithm:

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

Set $\Delta_{ij}^{(l)} = 0$ (for all l, i, j)

For $i=1$ to m

Set $a^{(1)} = x^{(i)}$

Perform forwar propagation to compute $a^{(l)}$ for $l = 1,2,3...,L$

Using $y^{(i)}$, compute $\delta^{(L)} = a^{(L)} - y^{(i)}$

Compute $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$

$\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Define $D_{ij}^{(l)} = \frac{\partial}{\partial \theta_{ij}^{(l)}} J(\theta) \Longleftrightarrow D_{ij}^{(l)} = \begin{cases} \frac{1}{m} \Delta_{ij}^{(l)} + \lambda \theta_{ij}^{(l)} & if\ j \neq 0 \\ \frac{1}{m} \Delta_{ij}^{(l)} & if\ j = 0 \end{cases}$

$\theta_{ij}^{(l)} := \theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$

Debugging Summary

To fix high variance(Overfitting):

1. Get more training examples.
2. Try a small sets of features.
3. Try increasing λ

To fix high bias(Underfitting):

1. Try get additional features.
2. Try adding polynomial features(x_1^2, x_2^2)
3. Try decreasing λ

Error metrics for skewed classes

Explanation for "skewed classes":

Train logistic regression model $h_\theta(x)$ ($y \in \{0, 1\}$). Find that you got 1% error on test set(99% correct). But, if the test set contains only 0.5% data which $y = 1$, the following function:

```
function y = predict(x);

y=0;

return;
```

gives a better error 0.5%. Such test set is called a "skewed class".

Error metrics

Actual class

Predicted class		1	0
	1	True positive	False positive
	0	False negative	True negative

$Precision = \frac{True\ positive}{True\ positive + False\ positive}$ （表示在被预测为1的样例中，真正是1的样例的个数）

$Recall = \frac{True\ positive}{True\ positive + False\ negative}$ （表示在所有真正是1的训练样例中，被预测为1的样例的个数）

Trading off precision and recall

Define threshhold:

Predict 1 if $h_\theta(x) \geq threshhold$, else predict 0.

Suppose we want to predict $y = 1$ only if very confident(high threshhold), it results in higher precision and lower recall.

Suppose we want to avoid missing too many cases of $y = 1$, it results in higher recall and lower precision.

How to choose threshhold?

Define:

$F_1\ Score = 2\frac{Precision \times Recall}{Precision + Recall}$ (also called $F\ Score$)

We wish to have an as high $F_1\ Score$ as possible.

Support Vector Machine(SVM)

Hypothesis

$h_\theta(x) = \begin{cases} 1 & if\, \theta^T x \geq 1 \\ 0 & if\, \theta^T x \leq -1 \end{cases}$

Cost Function

$J(\theta) = C \sum_{i=1}^{m} [\, y^{(i)} cost_1(\theta^T x^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T x^{(i)})\,] + \frac{1}{2} \sum_{i=1}^{n} \theta_j^2$

$cost_0(z) = \begin{cases} -z+1 & z<1 \\ 0 & z \geq 1 \end{cases}$

$cost_1(z) = \begin{cases} 0 & z<-1 \\ z+1 & z \geq -1 \end{cases}$

Predict $y = 1$ if $\theta^T x \geq 1$, and predict $y = 0$ if $\theta^T x \leq -1$.

Kernel

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

Choose $l^{(1)} = x^{(1)}, l^{(2)} = x^{(2)}, \ldots, l^{(m)} = x^{(m)}$

For training example $(x^{(i)}, y^{(i)})$:

Replace $x^{(i)}$ with: $f_0^{(i)} = 1$

$f_1^{(i)} = similarity(x^{(i)}, l^{(1)})$

$f_2^{(i)} = similarity(x^{(i)}, l^{(2)})$

$\ldots$

$f_m^{(i)} = similarity(x^{(i)}, l^{(m)})$

$$\implies f^{(i)} = \begin{bmatrix} f_0^{(i)} \\ f_1^{(i)} \\ f_2^{(i)} \\ \dots \\ f_m^{(i)} \end{bmatrix} \in R^{m+1} \ (f^{(i)} \text{ is the new feature.})$$

Predict $y = 1$ if $\theta^T f^{(i)} \geq 0$.

Function $similarity$ is called ***"Kernel"***.

Gaussian Kernel

$similarity(x, l) = e^{-\frac{\|x-l\|^2}{2\sigma^2}}$

Polynomial Kernel

$similarity(x, l) = (x^T l + C)^d$

Cost Function with Kernel

$J(\theta) = C \sum_{i=1}^{m} [\, y^{(i)} cost_1(\theta^T f^{(i)}) + (1 - y^{(i)}) cost_0(\theta^T f^{(i)}) \,] + \frac{1}{2} \sum_{j=1}^{m} \theta_j^2$