

# Machine Learning Formulas

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# 1 线性回归(Linear Regression)

## 1.1 当训练集X只有1项时

$$X = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{(n+1)*1} \quad (1)$$

$$\theta = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{pmatrix}_{(n+1)*1} \quad (2)$$

$$y = y \quad (3)$$

$$\begin{aligned} h_{\theta}(x) &= \theta^T X = X^T \theta \\ &= \begin{pmatrix} 1 & x_1 & x_2 & \dots & x_n \end{pmatrix} \begin{pmatrix} \theta_0 \\ \theta_1 \\ \dots \\ \theta_n \end{pmatrix} \\ &= \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n \end{aligned} \quad (4)$$

## 1.2 当训练集X有m项时

$$\begin{aligned}
 X &= \begin{pmatrix} x^{(1)} \\ x^{(2)} \\ x^{(3)} \\ \vdots \\ x^{(m)} \end{pmatrix} \\
 &= \begin{pmatrix} x_0^{(1)} & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ x_0^{(2)} & x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ x_0^{(3)} & x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ x_0^{(m)} & x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \\
 &= \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix}_{m \times (n+1)}
 \end{aligned} \tag{5}$$

$$\theta = \begin{pmatrix} \theta^{(0)} \\ \theta^{(1)} \\ \theta^{(2)} \\ \theta^{(3)} \\ \vdots \\ \theta^{(n)} \end{pmatrix}_{(n+1) \times 1} \tag{6}$$

$$y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{pmatrix}_{m \times 1} \tag{7}$$

### 1.2.1 Cost Function

1. 数值形式:

$$J(\theta) = \frac{1}{2m} [h_{\theta}(x^{(i)}) - y^{(i)}]^2 \tag{8}$$

2. 矩阵形式:

$$J(\theta) = \frac{1}{2m} [h_{\theta}(x) - y]^T [h_{\theta}(x) - y] \tag{9}$$

### 1.2.2 梯度下降

#### 1. 数值形式

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m} [h_{\theta}(x^{(i)}) - y^{(i)}] x_j^{(i)} \quad (10)$$

迭代方式:

$$\theta_j := \theta_j - \alpha \frac{1}{m} [h_{\theta}(x^{(i)}) - y^{(i)}] x_j^{(i)} \quad (11)$$

#### 2. 矩阵形式

$$\nabla J(\theta) = \frac{1}{2m} X^T [h_{\theta}(x) - y] \quad (12)$$

迭代方式:

$$\theta := \theta - \alpha \frac{1}{m} X^T [h_{\theta}(x) - y] \quad (13)$$

### 1.3 Feature Normalization

$$x_i = \frac{x_i - \mu}{\sigma} \quad (14)$$

或

$$x_i = \frac{x_i - \mu}{\max - \min} \quad (15)$$

### 1.4 公式法求解 (Normal Equation)

$$\theta = (X^T X)^{-1} X^T y \quad (16)$$

## 2 逻辑回归(Logistic Regression)

### 2.1 当只有2个类别时，使用1个分类器

#### 2.1.1 预测函数

##### 1. 数值形式

$$h_{\theta}(x) = \frac{1}{1 + e^{\theta^T x}} \quad (17)$$

##### 2. 矩阵形式

$$h_{\theta}(X) = \frac{1}{1 + e^{X\theta^T}} \quad (18)$$

#### 2.1.2 Cost Function

##### 1. 数值形式

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m [-y^{(i)} \log h_{\theta}(x^{(i)}) - (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)}))] \quad (19)$$

##### 2. 矩阵形式

$$J(\theta) = \frac{1}{m} [-y^T \log h_{\theta}(x) - (1 - y^T) \log(1 - h_{\theta}(x))] \quad (20)$$

#### 2.1.3 梯度下降

##### 1. 数值形式

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m} \sum_{i=1}^m [h_{\theta}(x^{(i)}) - y^{(i)}] x_j^{(i)} \quad (21)$$

迭代方式:

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m [h_{\theta}(x^{(i)}) - y^{(i)}] x_j^{(i)} \quad (22)$$

##### 2. 梯矩阵形式

$$\nabla J(\theta) = \frac{1}{m} X^T [h_{\theta}(x) - y] \quad (23)$$

迭代方式:

$$\theta := \theta - \alpha \frac{1}{m} X^T [h_{\theta}(x) - y] \quad (24)$$

## 2.2 当只有k个类别时，使用k个分类器

## 2.3 避免过拟合

### 1. 线性回归

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^m [h_{\theta}(x^{(i)}) - y^{(i)}]^2 + \lambda \frac{1}{2m} \sum_{j=1}^n \theta_j^2 \quad (25)$$

$$\theta_j = \theta_j (1 - \alpha \frac{\lambda}{m}) - \frac{\alpha}{m} \sum_{i=1}^n [h_{\theta}(x) - y] x_j^{(i)} \quad (26)$$

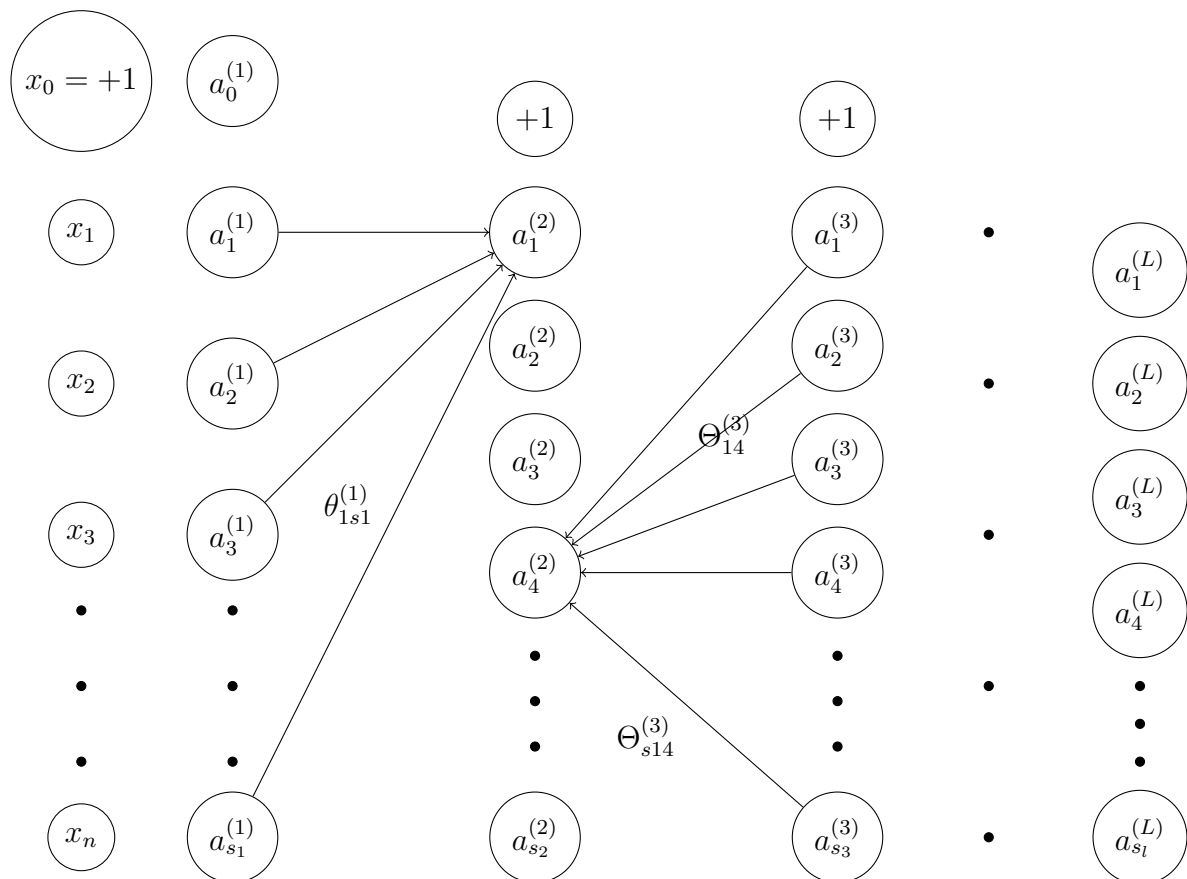
### 2. 逻辑回归

$$J(\theta) = \frac{1}{m} \sum_{i=1}^m [-y^{(i)} \log h_{\theta}(x^{(i)}) - (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)}))] + \lambda \frac{1}{2m} \sum_{j=1}^n \theta_j^2 \quad (27)$$

$$\theta_j = \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m [h_{\theta}(x^{(i)}) - y^{(i)}] x_j^{(i)} + \frac{\lambda}{m} \theta_j \right] \quad (28)$$

### 3 神经网络图例

#### 3.1 神经网络示意图





## 3.2 神经网络 – 前向算法

### 3.2.1 $X$ 、 $\theta$ 、 $\Theta$ 、 $z$ 、 $a$

1.  $X$

$$\begin{aligned}
 X &= \begin{pmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ (x^{(3)})^T \\ \vdots \\ (x^{(m)})^T \end{pmatrix} \\
 &= \begin{pmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \\
 &= \begin{pmatrix} x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \Rightarrow (m, n)
 \end{aligned} \tag{29}$$

2.  $a^{(1)}$

$$a^{(1)} = X \Rightarrow (m, n) \tag{30}$$

3.  $\Theta^{(1)}$

$$\Theta^{(1)} = \begin{pmatrix} \theta_{10}^{(1)} & \theta_{11}^{(1)} & \theta_{12}^{(1)} & \dots & \theta_{1,s_1}^{(1)} \\ \theta_{20}^{(1)} & \theta_{21}^{(1)} & \theta_{22}^{(1)} & \dots & \theta_{2,s_1}^{(1)} \\ \theta_{30}^{(1)} & \theta_{31}^{(1)} & \theta_{32}^{(1)} & \dots & \theta_{3,s_1}^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{s_2 0}^{(1)} & \theta_{s_2 1}^{(1)} & \theta_{s_2 2}^{(1)} & \dots & \theta_{s_2, s_1}^{(1)} \end{pmatrix} \Rightarrow (s_2, s_1 + 1) = (s_2, n + 1) \tag{31}$$

4.  $z^{(2)}$

给 $a^{(1)}$ 的每个数据均添加上 $a_0 = 1$ 后与 $\Theta^{(1)}$ 计算,得到 $z^{(2)\text{注}[1]} = (1, a^{(1)})(\Theta^{(1)})^T$

$$\begin{aligned}
z^{(2)} &= a^{(1)}(\Theta^{(1)})^T \Rightarrow (m, n+1) * (n+1, s_2) \\
&= \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \begin{pmatrix} \theta_{10}^{(1)} & \theta_{11}^{(1)} & \theta_{12}^{(1)} & \dots & \theta_{1,n}^{(1)} \\ \theta_{20}^{(1)} & \theta_{21}^{(1)} & \theta_{22}^{(1)} & \dots & \theta_{2,n}^{(1)} \\ \theta_{30}^{(1)} & \theta_{31}^{(1)} & \theta_{32}^{(1)} & \dots & \theta_{3,n}^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{s_2,0}^{(j)} & \theta_{s_2,1}^{(j)} & \theta_{s_2,2}^{(j)} & \dots & \theta_{s_2,n}^{(1)} \end{pmatrix}^T \\
&= \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & x_3^{(1)} & \dots & x_n^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & x_3^{(2)} & \dots & x_n^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} & x_3^{(3)} & \dots & x_n^{(3)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(m)} & x_2^{(m)} & x_3^{(m)} & \dots & x_n^{(m)} \end{pmatrix} \begin{pmatrix} \theta_{10}^{(1)} & \theta_{20}^{(1)} & \theta_{30}^{(1)} & \dots & \theta_{s_2,0}^{(1)} \\ \theta_{11}^{(1)} & \theta_{21}^{(1)} & \theta_{31}^{(1)} & \dots & \theta_{s_2,1}^{(1)} \\ \theta_{12}^{(1)} & \theta_{22}^{(1)} & \theta_{32}^{(1)} & \dots & \theta_{s_2,2}^{(1)} \\ \theta_{13}^{(1)} & \theta_{23}^{(1)} & \theta_{33}^{(1)} & \dots & \theta_{s_2,3}^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{1,n}^{(1)} & \theta_{2,n}^{(1)} & \theta_{3,n}^{(1)} & \dots & \theta_{s_2,n}^{(1)} \end{pmatrix} \\
&= \begin{pmatrix} z^{(2)(1)} \\ z^{(2)(2)} \\ z^{(2)(3)} \\ \vdots \\ z^{(2)(m)} \end{pmatrix} \\
&= \begin{pmatrix} z_1^{(2)(1)} & z_2^{(2)(1)} & z_3^{(2)(1)} & \dots & z_{s_2}^{(2)(1)} \\ z_1^{(2)(2)} & z_2^{(2)(2)} & z_3^{(2)(2)} & \dots & z_{s_2}^{(2)(2)} \\ z_1^{(2)(3)} & z_2^{(2)(3)} & z_3^{(2)(3)} & \dots & z_{s_2}^{(2)(3)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ z_1^{(2)(m)} & z_2^{(2)(m)} & z_3^{(2)(m)} & \dots & z_{s_2}^{(2)(m)\text{注}[2]} \end{pmatrix} \Rightarrow (m, n+1) * (n+1, s_2) = (m, s_2)
\end{aligned} \tag{32}$$

5.  $a^{(2)}$

$$a^{(2)} = g(z^{(2)}) \Rightarrow (m, s_2) \tag{33}$$

6. 一般式

<sup>注[1]</sup>从 $a^{(1)}$ 得到 $a^{(2)}$ 需要经过sigmoid()函数, 后续的从 $a^{(j)}$ 得到 $a^{(j+1)}$ 均需要经过sigmoid()函数

后续同理：

$$\begin{aligned}
\Theta^{(2)} &= \begin{pmatrix} \theta_{10}^{(2)} & \theta_{11}^{(2)} & \theta_{12}^{(2)} & \cdots & \theta_{1,s_2}^{(2)} \\ \theta_{20}^{(2)} & \theta_{21}^{(2)} & \theta_{22}^{(2)} & \cdots & \theta_{2,s_2}^{(2)} \\ \theta_{30}^{(2)} & \theta_{31}^{(2)} & \theta_{32}^{(2)} & \cdots & \theta_{3,s_2}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{s_3 0}^{(2)} & \theta_{s_3 1}^{(2)} & \theta_{s_3 2}^{(2)} & \cdots & \theta_{s_3, s_2}^{(2)} \end{pmatrix} \Rightarrow (s_3, s_2 + 1) \\
z^{(3)} &= (1, a^{(2)})(\Theta^{(2)})^T \Rightarrow (m, s_2 + 1) * (s_2 + 1, s_3) = (m, s_3) \\
a^{(3)} &= g(z^{(3)}) \Rightarrow (m, s_3) \\
&\vdots \\
a^{(j)} &= g(z^{(j-1)}) \Rightarrow (m, s_j) \\
\Theta^{(j)} &= \begin{pmatrix} \theta_{10}^{(j)} & \theta_{11}^{(j)} & \theta_{12}^{(j)} & \cdots & \theta_{1,s_j}^{(j)} \\ \theta_{20}^{(j)} & \theta_{21}^{(j)} & \theta_{22}^{(j)} & \cdots & \theta_{2,s_j}^{(j)} \\ \theta_{30}^{(j)} & \theta_{31}^{(j)} & \theta_{32}^{(j)} & \cdots & \theta_{3,s_j}^{(j)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{s_{j+1} 0}^{(j)} & \theta_{s_{j+1} 1}^{(j)} & \theta_{s_{j+1} 2}^{(j)} & \cdots & \theta_{s_{j+1}, s_j}^{(j)} \end{pmatrix} \Rightarrow (s_{j+1}, s_j + 1) \\
z^{(j+1)} &= (1, a^{(j)})(\Theta^{(j)})^T \Rightarrow (m, s_j + 1) * (s_j + 1, s_{j+1}) = (m, s_{j+1}) \\
a^{(j+1)} &= g(z^{(j+1)}) \Rightarrow (m, s_{j+1})
\end{aligned} \tag{34}$$

### 3.2.2 y

$$y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ y^{(3)} \\ \vdots \\ y^{(m)} \end{pmatrix}_{m \times 1} \tag{35}$$

为进行矩阵运算，要将其转化为如下形式：<sup>注[3]</sup>

$$y = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{m \times s_L} \tag{36}$$

<sup>注[3]</sup>y所对应的值所在的索引位置值为1，其他位置均为0