

① W_2, b_2 : 隐藏层 $\xrightarrow{\text{softmax}}$ 输出层 (\hat{y}) \rightarrow 监督数据 y

W_2 令 n 为特征个数, K 为目标分类个数 (在本题中, $n=256, K=10$), 则对于一个 $n \times 1$ 的输入样本向量 $x^{(i)} = (x_1^{(i)} \dots x_n^{(i)})^T$; 一个 $n \times K$ 的权重矩阵 W_2 , 及一个 $K \times 1$ 的偏置向量 b_2 , $z = W_2^T x^{(i)} + b_2$, $z_j = \sum_{i=1}^n W_{j,i} x_i^{(i)} + b_j$
 \hat{y} 与 y 均为 $K \times 1$ 的向量, $\hat{y}_j = \text{softmax}(z)_j = \frac{\exp(z_j)}{\sum_{q=1}^K \exp(z_q)}$

不考虑正则化时, $\text{Loss}(\hat{y}, y) = -\sum y_j \log(\hat{y}_j) = -\log(\hat{y}_t)$ (t 为正确分类)

$$\frac{\partial L}{\partial z_t} = \frac{\partial L}{\partial \hat{y}_t} \cdot \frac{\partial \hat{y}_t}{\partial z_t}, \text{ 其中, } \frac{\partial L}{\partial \hat{y}_t} = -\frac{1}{\hat{y}_t}$$

$$\text{对 } \frac{\partial \hat{y}_t}{\partial z_t} = \frac{\partial \text{softmax}(z)_t}{\partial z_t} = \frac{\exp(z_t) \sum \exp(z_q) - \exp(z_t)^2}{(\sum \exp(z_q))^2} = \hat{y}_t (1 - \hat{y}_t)$$

1° $j \neq t$

$$\frac{\partial L}{\partial z_t} = -\frac{1}{\hat{y}_t} \cdot \hat{y}_t (1 - \hat{y}_t) = \hat{y}_t - 1$$

2° $j = t$

$$\frac{\partial \hat{y}_t}{\partial z_j} = \exp(z_t) \frac{\partial (\frac{1}{\sum \exp(z_q)})}{\partial z_j} = -\hat{y}_t \cdot \hat{y}_j$$

$$\frac{\partial L}{\partial z_t} = -\frac{1}{\hat{y}_t} \cdot (-\hat{y}_t \cdot \hat{y}_j) = \hat{y}_j$$

$$\therefore \frac{\partial L}{\partial z} = [\hat{y}_1, \hat{y}_2, \dots, \hat{y}_{t-1}, \dots, \hat{y}_K] = \hat{y} - y$$

$$\therefore \frac{\partial L}{\partial W_i} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial W_i} = (\hat{y} - y) x_i^{(i)}$$

即 $\frac{\partial L}{\partial W_2} = (\hat{y} - y) x^{(i)}$, 其中 \hat{y} 是最终输出, y 是监督数据, $x^{(i)}$ 是隐藏层到监督层的输入

此时将样本量与 L_2 正则项纳入考虑, 设样本量为 m

$$\frac{\partial L}{\partial W_2} = (\hat{Y} - Y) X^{(1)}/m + \frac{\partial L}{\partial L_2} = (\hat{Y} - Y) X^{(1)} + \frac{\partial L}{\partial \left(\frac{\lambda}{2m} \left(\sum_{i=1}^k W_i^T W_i \right) \right)}$$

$$= (\hat{Y} - Y) X^{(1)}/m + \frac{\lambda}{m} W_2$$

$$\boxed{b_2} \quad \frac{\partial L}{\partial b_2} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial b_2} = \frac{\partial L}{\partial z} = (\hat{Y} - Y)/m$$

② W_1, b_1 : 输入层 $\xrightarrow{\text{ReLU}}$ 隐藏层

$\boxed{W_1}$ 设输入向量为 $X^{(0)} = (X_1^{(0)}, \dots, X_n^{(0)})^T$, 权重矩阵 W_1 为 $n \times n$, 偏置向量 b_1 为 $n \times 1$, $h = W^T X^{(0)} + b$, $h_j = \sum_{i=1}^n W_{j,i} X_i^{(0)} + b_j$
 $X^{(1)}$ 是 h 经 ReLU 函数后的输出, $X_j^{(1)} = \max(0, h_j)$

$$\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial h} \cdot \frac{\partial h}{\partial W_1} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial X^{(1)}} \cdot \frac{\partial X^{(1)}}{\partial h} \cdot \frac{\partial h}{\partial W_1}$$

$$\frac{\partial L}{\partial z} = \hat{Y} - Y, \quad \frac{\partial z}{\partial X^{(1)}} = W_2^T$$

$$\frac{\partial X^{(1)}}{\partial h_j} = \begin{cases} 0, & 0 \geq h_j \\ 1, & 0 < h_j \end{cases} \quad \frac{\partial h}{\partial W_1} = X^{(0)}$$

$$\therefore \frac{\partial L}{\partial W_1} = ((\hat{Y} - Y) W_2^T X^{(1)*})/m, \text{ 其中对 } X^{(1)*} \text{ 中的每一个样本 } X_j^{(1)*},$$

$$X_{j,i}^{(1)*} = \begin{cases} 0, & 0 \geq h_i = \sum_k W_{i,k} X_{j,k}^{(0)} + b_i \\ X_{j,i}^{(0)}, & 0 < h_i = \sum_k W_{i,k} X_{j,k}^{(0)} + b_i \end{cases}$$

$$\text{加上正则项的梯度后, } \frac{\partial L}{\partial W_{1,i}} = \left((\hat{Y} - Y) W_2^T X^{(1)*} \right) / m + \frac{\lambda}{m} W_1$$

($X^{(1)*}$ 如上定义)

b1

$$\frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial z} \cdot \frac{\partial z}{\partial X^{(1)}} \cdot \frac{\partial X^{(1)}}{\partial h} \cdot \frac{\partial h}{\partial b_1}$$

$$= ((\hat{Y} - Y) \cdot W_2^T \cdot 1^*) / n, \text{ 其中 } 1^*_i = \begin{cases} 0, & 0 \geq h_i \\ 1, & 0 < h_i \end{cases}$$