如图所示三层神经网络:输入层 $Layer_1$ 、隐含层 $Layer_2$ 、输出层 $Layer_3$.输入层包括三个神经元,即输入为 $\mathbf{x} = \{x_1, x_2, x_3\}$,样本数据集为 $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}$,目标输出为 o_1^{T} 和 o_2^{T} . $\omega_{ij}^{\mathrm{L}_k}$ 为第 k-1 层的第 i 个神经元到第 k 层的第 j 个神经元之间的权重。 $\mathbf{b}^{\mathrm{L}_k} = \{b_i^{\mathrm{L}_k}\}$ 为第 k 层神经元偏移量集合, $b_j^{\mathrm{L}_k}$ 为第 k 层第 i 个神经元的偏移量。 $net_i^{\mathrm{L}_k}$ 表示第 k 层网络的第 i 个神经元的输入, $o_i^{\mathrm{L}_k}$ 表示第 k 层网络的第 i 个神经元的激活函数。

假设激活函数为 sigmoid 函数:

$$f(x) = \frac{1}{1 + e^{-x}} \tag{1}$$

其导数为:

$$f'(x) = f(x)(1 - f(x))$$
 (2)

对于 $Layer_2$ 层第 i 个神经元的输出:

$$net_j^{L_2} = \sum_{i=1}^3 \omega_{ij}^{L_1} \times x_i + b_j^{L_2}$$
 (3)

对于 $Layer_3$ 层的第 j 个神经元的输出:

$$net_j^{\mathcal{L}_3} = \sum_{i=1}^2 \omega_{ij}^{\mathcal{L}_2} \times o_i^{\mathcal{L}_2} + b_j^{\mathcal{L}_3}$$
 (4)

第 L_i 层的第 j 个神经元的输出:

$$o_j^{\mathcal{L}_i} = f_j^{\mathcal{L}_i}(net_j^{\mathcal{L}_i}) = \frac{1}{1 + e^{-net_j^{\mathcal{L}_i}}}$$
 (5)

输出的总误差为:

$$E_{\text{Total}} = \frac{1}{2} \sum_{i=1}^{2} (o_j^{\text{T}} - o_j^{\text{L}_3})^2 = \frac{1}{2} ((o_1^{\text{T}} - o_1^{\text{L}_3})^2 + (o_2^{\text{T}} - o_2^{\text{L}_3})^2)$$
 (6)

是 $o_1^{L_3}$ 和 $o_2^{L_3}$ 的函数

1 Layer₂ 与 Layer₃ 间参数调整

调整 $Layer_2$ 与 $Layer_3$ 间的权重 $\omega_{ij}^{L_2}$

$$\frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{\text{L}_2}} = \frac{\partial E_{\text{Total}}}{\partial o_i^{\text{L}_3}} \cdot \frac{\partial o_j^{\text{L}_3}}{\partial net_j^{\text{L}_3}} \cdot \frac{\partial net_j^{\text{L}_3}}{\partial \omega_{ij}^{\text{L}_2}}$$
(7)

$$= -(o_j^{\mathrm{T}} - o_j^{\mathrm{L_3}}) \cdot f_j^{\mathrm{L_3}}(net_j^{\mathrm{L_3}})(1 - f_j^{\mathrm{L_3}}(net_j^{\mathrm{L_3}})) \cdot o_i^{\mathrm{L_2}}$$
(8)

$$= -(o_j^{\mathrm{T}} - o_j^{\mathrm{L}_3}) \cdot o_j^{\mathrm{L}_3} (1 - o_j^{\mathrm{L}_3}) \cdot o_i^{\mathrm{L}_2}$$
(9)

(10)

令 $\delta^{\mathbf{L}_2}_{ij}$ 表示 $Layer_2$ 层第 i 个神经元与 $Layer_3$ 层第 j 个神经元间权重的梯度项,则

$$\delta_{ij}^{L_2} = \frac{\partial E_{\text{Total}}}{\partial o_j^{L_3}} \cdot \frac{\partial o_j^{L_3}}{\partial net_j^{L_3}} \tag{11}$$

$$= -(o_j^{\mathrm{T}} - o_j^{\mathrm{L_3}}) \cdot o_j^{\mathrm{L_3}} (1 - o_j^{\mathrm{L_3}}) \tag{12}$$

可以看出, $Layer_2$ 层第 i 个神经元与 $Layer_3$ 层第 j 个神经元间权重的梯度项是与 i 无关的,故连接至 $Layer_3$ 层第 j 个神经元相对应的权重的梯度向均为 $\delta_{ij}^{L_2}$,用 $\delta_{ij}^{L_2}$ 表示,

$$\delta_{\cdot j}^{\mathcal{L}_2} = \delta_{ij}^{\mathcal{L}_2} = -(o_j^{\mathcal{T}} - o_j^{\mathcal{L}_3}) \cdot o_j^{\mathcal{L}_3} (1 - o_j^{\mathcal{L}_3}) \tag{13}$$

则整体误差 $E_{ ext{Total}}$ 对 $\omega_{ij}^{ extsf{L}_2}$ 的偏导数公式写作:

$$\frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{\text{L}_2}} = \delta_{\cdot j}^{\text{L}_2} \cdot o_i^{\text{L}_2} \tag{14}$$

则权重 $\omega_{ij}^{L_2}$ 的学习公式为:

$$\widehat{\omega}_{ij}^{L_2} = \omega_{ij}^{L_2} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{L_2}} = \omega_{ij}^{L_2} - \eta \cdot \delta_{\cdot j}^{L_2} \cdot o_i^{L_2}$$
(15)

η为学习速率

 $Layer_3$ 的第 i 个神经元的偏移量的梯度为

$$\frac{\partial E_{\text{Total}}}{\partial b_j^{\text{L}_3}} = \frac{\partial E_{\text{Total}}}{\partial o_j^{\text{L}_3}} \cdot \frac{\partial o_j^{\text{L}_3}}{\partial net_j^{\text{L}_3}} \cdot \frac{\partial net_j^{\text{L}_3}}{\partial b_j^{\text{L}_3}}$$
(16)

$$= -(o_i^{\mathrm{T}} - o_i^{\mathrm{L}_3}) \cdot f_i^{\mathrm{L}_3}(net_i^{\mathrm{L}_3})(1 - f_i^{\mathrm{L}_3}(net_i^{\mathrm{L}_3})) \cdot 1 \tag{17}$$

$$= -(o_i^{\mathrm{T}} - o_i^{\mathrm{L_3}}) \cdot o_i^{\mathrm{L_3}} (1 - o_i^{\mathrm{L_3}}) \tag{18}$$

$$=\delta^{\mathcal{L}_2}_{\cdot j} \tag{19}$$

偏移 $b_i^{L_3}$ 的学习公式为:

$$\hat{b}_j^{\mathcal{L}_3} = b_j^{\mathcal{L}_3} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial b_i^{\mathcal{L}_3}} = b_j^{\mathcal{L}_3} - \eta \cdot \delta_{\cdot j}^{\mathcal{L}_2}$$
(20)

例如,对于权重 $\omega_{11}^{L_2}$ 的更新学习公式为:

$$\widehat{\omega}_{11}^{L_2} = \omega_{11}^{L_2} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{L_2}}$$
(21)

$$=\omega_{11}^{L_2} - \eta \cdot \delta_{11}^{L_2} \cdot o_1^{L_2} \tag{22}$$

$$= \omega_{11}^{L_2} - \eta \cdot \left(- \left(o_1^{T} - o_1^{L_3} \right) \cdot o_1^{L_3} (1 - o_1^{L_3}) \right) \cdot o_1^{L_2}$$
 (23)

$$= \omega_{11}^{L_2} + \eta \cdot (o_1^{T} - o_1^{L_3}) \cdot o_1^{L_3} (1 - o_1^{L_3}) \cdot o_1^{L_2}$$
(24)

例如,对于偏移 $b_1^{L_3}$ 的更新学习公式为:

$$\hat{b}_{1}^{\mathrm{L}_{3}} = b_{1}^{\mathrm{L}_{3}} - \eta \cdot \frac{\partial E_{\mathrm{Total}}}{\partial b_{1}^{\mathrm{L}_{3}}} \tag{25}$$

$$= b_1^{L_3} + \eta \cdot (o_1^{T} - o_1^{L_3}) \cdot o_1^{L_3} (1 - o_1^{L_3})$$
(26)

2 Layer₁ 与 Layer₂ 间参数调整

调整 $Layer_1$ 与 $Layer_2$ 间的权重 $\omega_{ij}^{L_1}$

$$\frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{\text{L}_1}} = \left(\sum_{k=1}^{2} \frac{\partial E_{\text{Total}}}{\partial o_k^{\text{L}_3}} \frac{\partial o_k^{\text{L}_3}}{\partial net_k^{\text{L}_3}} \frac{\partial net_k^{\text{L}_3}}{\partial o_j^{\text{L}_2}}\right) \cdot \frac{\partial o_j^{\text{L}_2}}{\partial net_j^{\text{L}_2}} \cdot \frac{\partial net_j^{\text{L}_2}}{\partial \omega_{ij}^{\text{L}_1}}$$
(27)

$$= \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\text{Layer}_{2}} \omega_{3k}^{\text{L}_{2}}\right) \cdot f_{j}^{\text{L}_{2}} (net_{j}^{\text{L}_{2}}) (1 - f_{j}^{\text{L}_{2}} (net_{j}^{\text{L}_{2}})) \cdot x_{i}$$
 (28)

$$= \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\text{Layer}_{2}} \omega_{3k}^{\text{L}_{2}}\right) \cdot o_{j}^{\text{L}_{2}} (1 - o_{j}^{\text{L}_{2}}) \cdot x_{i}$$
(29)

(30)

令 $\delta_{ij}^{\mathbf{L}_1}$ 表示 $Layer_1$ 层第 i 个神经元与 $Layer_2$ 层第 j 个神经元间权重的梯度项,则

$$\delta_{ij}^{L_1} = \left(\sum_{k=1}^{2} \frac{\partial E_{\text{Total}}}{\partial o_k^{L_3}} \frac{\partial o_k^{L_3}}{\partial net_k^{L_3}} \frac{\partial net_k^{L_3}}{\partial o_j^{L_2}}\right) \cdot \frac{\partial o_j^{L_2}}{\partial net_j^{L_2}}$$
(31)

$$= \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\text{Layer}_{2}} \omega_{3k}^{\text{L}_{2}}\right) \cdot o_{j}^{\text{L}_{2}} (1 - o_{j}^{\text{L}_{2}})$$
(32)

可以看出, $Layer_1$ 层第 i 个神经元与 $Layer_2$ 层第 j 个神经元间权重的梯度项是与 i 无关的,故连接至 $Layer_2$ 层第 j 个神经元相对应的权重的梯度向均为 $\delta_{ij}^{L_1}$,用 $\delta_{ij}^{L_1}$ 表示,

$$\delta_{\cdot j}^{\mathcal{L}_{1}} = \delta_{ij}^{\mathcal{L}_{1}} = \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\mathcal{L}_{ayer_{2}}} \omega_{3k}^{\mathcal{L}_{2}}\right) \cdot o_{j}^{\mathcal{L}_{2}} (1 - o_{j}^{\mathcal{L}_{2}})$$
(33)

则整体误差 E_{Total} 对 $\omega_{ij}^{\text{L}_1}$ 的偏导数公式写作:

$$\frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{\text{L}_1}} = \delta_{.j}^{\text{L}_1} \cdot x_i \tag{34}$$

则权重 $\omega_{ij}^{L_1}$ 的学习公式为:

$$\widehat{\omega}_{ij}^{\mathcal{L}_1} = \omega_{ij}^{\mathcal{L}_1} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial \omega_{ij}^{\mathcal{L}_1}} = \omega_{ij}^{\mathcal{L}_1} - \eta \cdot \delta_{\cdot j}^{\mathcal{L}_1} \cdot x_i$$
(35)

$$\frac{\partial E_{\text{Total}}}{\partial b_{i}^{\text{L}_{2}}} = \left(\sum_{k=1}^{2} \frac{\partial E_{\text{Total}}}{\partial o_{k}^{\text{L}_{3}}} \frac{\partial o_{k}^{\text{L}_{3}}}{\partial net_{k}^{\text{L}_{3}}} \frac{\partial net_{k}^{\text{L}_{3}}}{\partial o_{i}^{\text{L}_{2}}}\right) \cdot \frac{\partial o_{j}^{\text{L}_{2}}}{\partial net_{j}^{\text{L}_{2}}} \cdot \frac{\partial net_{j}^{\text{L}_{2}}}{\partial b_{i}^{\text{L}_{2}}}$$
(36)

$$= \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\text{Layer}_{2}} \omega_{3k}^{\text{L}_{2}}\right) \cdot f_{j}^{\text{L}_{2}}(net_{j}^{\text{L}_{2}}) \left(1 - f_{j}^{\text{L}_{2}}(net_{j}^{\text{L}_{2}})\right) \cdot 1 \tag{37}$$

$$= \left(\sum_{k=1}^{2} \delta_{\cdot k}^{\text{Layer}_{2}} \omega_{3k}^{\text{L}_{2}}\right) \cdot o_{j}^{\text{L}_{2}} (1 - o_{j}^{\text{L}_{2}})$$
(38)

$$= \delta_{\cdot j}^{\mathcal{L}_1} \tag{39}$$

偏移 $b_i^{L_2}$ 的学习公式为:

$$\hat{b}_j^{\mathcal{L}_2} = b_j^{\mathcal{L}_2} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial b_i^{\mathcal{L}_2}} = b_j^{\mathcal{L}_2} - \eta \cdot \delta_{\cdot j}^{\mathcal{L}_1}$$

$$\tag{40}$$

例如,对于权重 $\omega_{23}^{\rm L_1}$ 的更新学习公式为:

$$\widehat{\omega}_{23}^{\mathcal{L}_1} = \omega_{23}^{\mathcal{L}_2} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial \omega_{23}^{\mathcal{L}_1}} \tag{41}$$

$$=\omega_{23}^{\mathcal{L}_{2}}-\eta\cdot \Big((\sum_{j=1}^{2}\frac{\partial E_{\text{Total}}}{\partial o_{j}^{\mathcal{L}_{3}}}\frac{\partial o_{j}^{\mathcal{L}_{3}}}{\partial net_{j}^{\mathcal{L}_{3}}}\frac{\partial net_{j}^{\mathcal{L}_{3}}}{\partial o_{3}^{\mathcal{L}_{2}}})\cdot \frac{\partial o_{3}^{\mathcal{L}_{2}}}{\partial net_{3}^{\mathcal{L}_{2}}}\cdot \frac{\partial net_{3}^{\mathcal{L}_{2}}}{\partial \omega_{23}^{\mathcal{L}_{1}}}\Big) \tag{42}$$

$$= \omega_{23}^{L_2} - \eta \cdot \left(\sum_{j=1}^{2} \delta_{\cdot j}^{\text{Layer}_2} \omega_{3j}^{L_2}\right) \cdot f_3^{L_2} (net_3^{L_2}) (1 - f_3^{L_2} (net_3^{L_2})) \cdot x_2$$
 (43)

$$= \omega_{23}^{L_2} - \eta \cdot \left(\sum_{j=1}^{2} \delta_{j}^{Layer_2} \omega_{3j}^{L_2}\right) \cdot o_3^{L_2} (1 - o_3^{L_2}) \cdot x_2 \tag{44}$$

例如,对于偏移 $b_3^{L_2}$ 的更新学习公式为:

$$\hat{b}_3^{L_2} = b_1^{L_3} - \eta \cdot \frac{\partial E_{\text{Total}}}{\partial b_3^{L_2}} \tag{45}$$

$$=b_{3}^{\mathbf{L}_{2}}-\eta\cdot \left(\left(\sum_{j=1}^{2}\frac{\partial E_{\mathrm{Total}}}{\partial o_{j}^{\mathbf{L}_{3}}}\frac{\partial o_{j}^{\mathbf{L}_{3}}}{\partial net_{j}^{\mathbf{L}_{3}}}\frac{\partial net_{j}^{\mathbf{L}_{3}}}{\partial o_{3}^{\mathbf{L}_{2}}}\right)\cdot \frac{\partial o_{3}^{\mathbf{L}_{2}}}{\partial net_{3}^{\mathbf{L}_{2}}}\cdot \frac{\partial net_{3}^{\mathbf{L}_{2}}}{\partial b_{3}^{\mathbf{L}_{2}}}\right) \tag{46}$$

$$= b_3^{L_2} - \eta \cdot (\sum_{i=1}^{2} \delta_{.j}^{Layer_2} \omega_{3j}^{L_2}) \cdot f_3^{L_2} (net_3^{L_2}) (1 - f_3^{L_2} (net_3^{L_2})) \cdot 1$$
(47)

$$= \omega_{23}^{L_2} - \eta \cdot \left(\sum_{j=1}^{2} \delta_{.j}^{\text{Layer}_2} \omega_{3j}^{L_2}\right) \cdot o_3^{L_2} (1 - o_3^{L_2})$$
(48)