

机器学习第二次作业

专业：计算机科学与技术

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一、实验要求

在这个练习中，你需要以三层感知机为例，使用反向传播算法更新MLP的权重和偏置项，并将推导过程以报告的形式提交。

MLP以及权重、偏置项的定义如下：

Define S_w and S_b as:

$$\begin{aligned} S_w &= \sum_{c=1}^C \sum_{\mathbf{y}_i^M \in c} (\mathbf{y}_i^M - \mathbf{m}_c^M)(\mathbf{y}_i^M - \mathbf{m}_c^M)^T \\ S_b &= \sum_{c=1}^C n_c (\mathbf{m}_c^M - \mathbf{m}^M)(\mathbf{m}_c^M - \mathbf{m}^M)^T \end{aligned} \quad (1)$$

where \mathbf{m}_c^M is the mean vector of \mathbf{y}_i^M (the output of the i th sample from the c th class), \mathbf{m}^M is the mean vector of the output \mathbf{y}_i^M from all classes, n_c is the number of samples from the c th class. Define the discriminative regularization term $tr(S_w) - tr(S_b)$ and incorporate it into the objective function of the MLP:

$$E = \sum_i \sum_j \frac{1}{2} (\mathbf{y}_{i,j}^M - \mathbf{d}_{i,j})^2 + \frac{1}{2} \gamma (tr(S_w) - tr(S_b)). \quad (2)$$

where $\mathbf{y}_{i,j}^M$ is the j th element in the vector \mathbf{y}_i^M , $\mathbf{d}_{i,j}$ is the j th element in the label vector \mathbf{d}_i , tr denotes the trace of the matrix. Use the BP algorithm to update parameters \mathbf{W} and \mathbf{b} of the MLP.

二、三层感知机

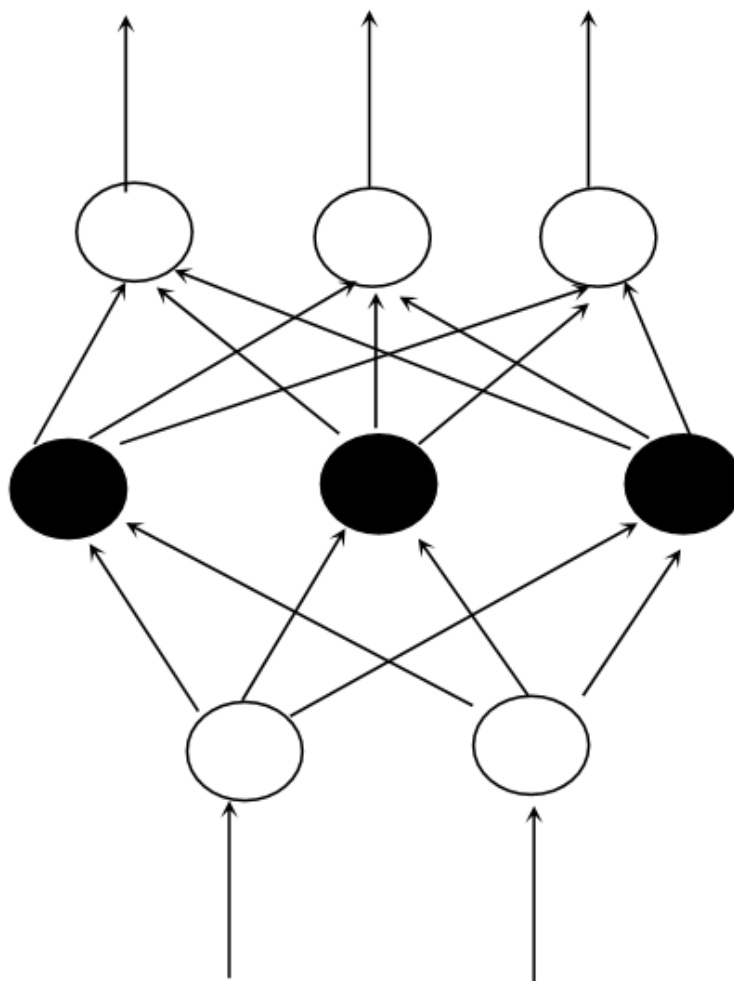
输出向量

输出层

隐藏层

输入层

输入向量



$$\text{权重矩阵 } S_w = \sum_{c=1}^C \sum_{y_i^M \in c} (y_i^M - m_c^M)(y_i^M - m_c^M)^T$$

$$\text{偏置项矩阵 } S_b = \sum_{c=1}^C n_c (m_c^M - m^M)(m_c^M - m^M)^T$$

$$\text{误差评估函数 } E = \sum_i \sum_j \frac{1}{2} (y_{i,j}^M - d_{i,j})^2 + \frac{1}{2} \gamma (tr(S_w) - tr(S_b))$$

三、反向传播算法更新MLP的权重和偏置项

输出层权重与偏置更新

权重更新

$$\begin{aligned}\Delta W_{ij}^2 &= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial W_{ij}^2} \right) \\&= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial net_{ki}^2} \cdot \frac{\partial net_{ki}^2}{\partial W_{ij}^2} \right) \\&= - \sum_{k=0}^{n-1} \eta \frac{\partial E}{\partial out_{ki}^2} \cdot \frac{\partial out_{ki}^2}{\partial net_{ki}^2} \cdot \frac{\partial net_{ki}^2}{\partial W_{ij}^2} \\&= - \sum_{k=0}^{n-1} \frac{\partial E}{\partial out_{ki}^2} \cdot \eta \cdot out_{ki}^2 (1 - out_{ki}^2) \cdot out_{ki}^1 \\&= - \sum_{k=0}^{n-1} \eta \epsilon_{ki} \cdot out_{ki}^2 (1 - out_{ki}^2) \cdot out_{ki}^1\end{aligned}$$

偏置更新

$$\begin{aligned}\Delta b_i^2 &= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial b_i^2} \right) \\&= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial net_{ki}^2} \cdot \frac{\partial net_{ki}^2}{\partial b_i^2} \right) \\&= - \sum_{k=0}^{n-1} \eta \frac{\partial E}{\partial out_{ki}^2} \cdot \frac{\partial out_{ki}^2}{\partial net_{ki}^2} \cdot \frac{\partial net_{ki}^2}{\partial b_i^2} \\&= - \sum_{k=0}^{n-1} \frac{\partial E}{\partial out_{ki}^2} \cdot \eta \cdot out_{ki}^2 (1 - out_{ki}^2) \\&= - \sum_{k=0}^{n-1} \eta \epsilon_{ki} \cdot out_{ki}^2 (1 - out_{ki}^2)\end{aligned}$$
$$\begin{aligned}\epsilon_{ki} &= \frac{\partial E}{\partial net_{ki}^2} \\&= 2(out_{ki}^2 - d_{ki}) + \frac{1}{2}\gamma \left(\frac{\partial \text{Tr}(S_w)}{\partial out_{ki}^2} - \frac{\partial (\text{Tr}(S_b))}{\partial out_{ki}^2} \right)\end{aligned}$$

而：

$$\begin{aligned}
\frac{1}{2} \cdot \frac{\partial \text{Tr}(S_w)}{\partial out_{ki}^2} &= \left(1 - \frac{1}{n_c}\right) (out_{ki}^2 - m_{ci}^M) + \sum_{p=0, p \neq k}^{n_c-1} -\frac{1}{n_c} (y_{pi}^2 - m_{ci}^M) \\
&= out_{ki}^2 - m_{ci}^M + \sum_{p=0}^{n_c-1} -\frac{1}{n_c} (y_{pi}^2 - m_{ci}^M) \\
&= out_{ki}^2 - m_{ci}^M + \left(-\frac{1}{n_c}\right) (n_c m_{ci}^M - n_c m_{ci}^M) \\
&= out_{ki}^2 - m_{ci}^M
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2} \cdot \frac{\partial (\text{Tr}(S_b))}{\partial out_{ki}^2} &= n_c \left(\frac{1}{n_c} - \frac{1}{n}\right) (m_{ci}^M - m_i^M) + \sum_{p=0, p \neq c}^{C-1} -\frac{n_p}{n} (m_{pi}^M - m_i^M) \\
&= (m_{ci}^M - m_i^M) + \sum_{p=0}^{c-1} -\frac{n_p}{n} (m_{pi}^M - m_i^M) \\
&= (m_{ci}^M - m_i^M) + \left(-\frac{1}{n}\right) (n m_i^M - n m_i^M) \\
&= m_{ci}^M - m_i^M
\end{aligned}$$

则：

$$\begin{aligned}
\varepsilon_{ki} &= 2(out_{ki}^2 - d_{ki}) + \gamma(out_{ki}^2 - m_{ci}^M) - \gamma(m_{ci}^M - m_i^M) \\
&= (2 + \gamma)out_{ki}^2 - 2d_{ki} - 2\gamma m_{ci}^M + \gamma m_i^M
\end{aligned}$$

相关变量（隐藏层同）：

学习率： η

第n层由k个向量计算得到的输出向量的第i个值(未经过激活函数)： net_{ki}^n

第n层由k个向量计算得到的输出向量的第i个值(经过激活函数)： out_{ki}^n

输出结果中属于c类的向量个数： n_c

$$m_{ci}^M = \frac{\sum_{k=0, y_k \in c}^{n_c-1} out_{ki}^2}{n_c}$$

$$\begin{aligned}
m_i^M &= \frac{\sum_{k=0}^{n-1} out_{ki}^2}{n} \\
&= \frac{\sum_{p=0}^{c-1} n_p m_{pi}^M}{n}
\end{aligned}$$

隐藏层权重与偏置更新

权重更新

$$\begin{aligned}\Delta W_{ij}^1 &= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial W_{ij}^1} \right) \\&= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial net_{ki}^1} \cdot \frac{\partial net_{ki}^1}{\partial W_{ij}^1} \right) \\&= - \sum_{k=0}^{n-1} \eta \frac{\partial E}{\partial out_{ki}^1} \cdot \frac{\partial out_{ki}^1}{\partial net_{ki}^1} \cdot \frac{\partial net_{ki}^1}{\partial W_{ij}^1} \\&= - \sum_{k=0}^{n-1} \eta \sum_{p=0}^{N_2-1} \delta_{kp}^2 \frac{\partial net_{kp}^2}{\partial out_{ki}^1} out_{ki}^0 out_{ki}^1 (1 - out_{ki}^1) \\&= -\eta \sum_{k=0}^{n-1} out_{ki}^0 out_{ki}^1 (1 - out_{ki}^1) \sum_{p=0}^{N_2-1} \delta_{kp}^2 W_{ij}^2\end{aligned}$$

偏置更新

$$\begin{aligned}\Delta b_i^1 &= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial b_i^1} \right) \\&= \sum_{k=0}^{n-1} \left(-\eta \frac{\partial E}{\partial net_{ki}^1} \cdot \frac{\partial net_{ki}^1}{\partial b_i^1} \right) \\&= - \sum_{k=0}^{n-1} \eta \frac{\partial E}{\partial out_{ki}^1} \cdot \frac{\partial out_{ki}^1}{\partial net_{ki}^1} \cdot \frac{\partial net_{ki}^1}{\partial b_i^1} \\&= - \sum_{k=0}^{n-1} \eta \sum_{p=0}^{N_2-1} \delta_{kp}^2 \frac{\partial net_{kp}^2}{\partial out_{ki}^1} out_{ki}^1 (1 - out_{ki}^1) \\&= -\eta \sum_{k=0}^{n-1} out_{ki}^1 (1 - out_{ki}^1) \sum_{p=0}^{N_2-1} \delta_{kp}^2 W_{ij}^2\end{aligned}$$

其中：

$$\delta_{ki}^2 = \varepsilon_{ki} out_{ki}^2 (1 - out_{ki}^2)$$

更新方式

依据上面计算所得，我们可以如下更新权重和偏置：

$$W_{ij}^{n'} = W_{ij}^n + \Delta W_{ij}^n$$

$$b_i^{n'} = b_i^n + \Delta b_i^n$$