BACKPROPAGATION

一、内容

本部分将实现Dense Layer、Activation Function和Loss的反向传播。

二、代码

一、Dense Layer

公式

$$y = wx + b$$

$$\frac{\partial y}{\partial w} = x$$

$$\frac{\partial y}{\partial x} = w$$

$$\frac{\partial y}{\partial b} = 1$$

其中x是输入向量，w是权重，b是偏置，y是Dense Layer层是输出向量，b和w已经在初始化时保存，所以在前向传播中要将x保存在Dense Layer的属性中，**注意：1和w一样是一个矩阵，但大小不一样。**相关代码如下：

实现

```
def forward(self, input):
    # 因为要增加backward方法,
    # Layer_Dense的输出对输入（input）的偏导是self.weight,
    # 面Layer_Dense的输出对self.weight的偏导是输入（input）
    # 所以要在forward中增加self.input属性
    self.input = input #self.input是相对前面代码版本中新加入的
    self.output = np.dot(input, self.weight) + self.bias
```

公式

$$loss = f(y)$$

$$\frac{\partial loss}{\partial y} = dvalue$$

$$\frac{\partial loss}{\partial w} = \frac{\partial loss}{\partial y}\frac{\partial y}{\partial w} = dvalue * \frac{\partial y}{\partial w} = dvalue * x$$

$$\frac{\partial loss}{\partial x} = \frac{\partial loss}{\partial y}\frac{\partial y}{\partial x} = dvalue * \frac{\partial y}{\partial x} = dvalue * w$$

$$\frac{\partial loss}{\partial b} = \frac{\partial loss}{\partial y}\frac{\partial y}{\partial b} = dvalue * \frac{\partial y}{\partial b} = dvalue * 1$$

其中的dvalue通过下一层的反向传播求得，并作为这一层backward方法的参数，所以dvalue在该层中是已知的，只需通过代码实现求 $\frac{\partial y}{\partial w}$ 和 $\frac{\partial y}{\partial x}$ ，即 x 和 w ，代码如下:

实现

```
def backward(self, dvalue):
    # dvalue是loss对下一层（Activation）的输入（input）的导数,
    # 也就是loss对这一层（Layer_Dense）的输出（output）的导数,
    # 这里会用到链式法则

    # 在本层中，希望求得的是loss对这一层（Layer_Dense）的self.weight的导数
    # 这便找到了self.weight优化的方向（negative gradient direction）

    # 这里要考虑到self.dweight的大小要与self.weight一致，因为方便w - lr * dw公式进行优化
    # 假设input只有一个sample，大小为1xa，weight大小为axb，则output大小为1xb,
    # 因为loss是标量，所以dvalue = dloss/doutput大小即为output的大小(1xb),
    # 所以dweight的大小为(1xa).T * (1xb) = axb,大小和weight一致。
    # 注意：当input有多个sample时（一个矩阵输入），则dweight为多个axb矩阵相加。
```

```python
        self.dweight = np.dot(self.input.T, dvalue)

        # 在本层中，希望求得的是loss对这一层（Layer_Dense）的self.input的导数
        # 以便作为下一层的backward方法中的dvalue参数，

        # 因为loss是标量，所以dinput大小即为intput的大小(1xa)，
        # dvalue = dloss/doutput大小即为output的大小(1xb)，
        # weight大小为axb
        # 所以1xa = (1xb) * (axb).T
        self.dinput = np.dot(dvalue, self.weight.T)

        # 像self.dinput一样，self.dbias可以通过矩阵乘法实现，
        # self.dbias = np.dot( dvalue, np.ones( ( len(self.bias), len(self.bias) ) ) )
        # 但有更快更简单的实现
        self.dbias = np.sum(dvalue, axis=0, keepdims=True)# 此处不要keepdims=True也行，因为按0维相
加还是行向量
```

二、ReLu

公式

$$y = \begin{cases} x, x > 0 \\ 0, x \leq 0 \end{cases}$$

$$\frac{dy}{dx} = \begin{cases} 1, x > 0 \\ 0, x < 0 \end{cases}$$

$$loss = f(y)$$

$$\frac{\partial loss}{\partial x} = \frac{\partial loss}{\partial y}\frac{\partial y}{\partial x} = dvalue * \frac{\partial y}{\partial x} = \begin{cases} dvalue, x > 0 \\ 0, x < 0 \end{cases}$$

> 从矩阵的角度看 $\dfrac{\partial y}{\partial x}$ 是一个对角方阵，对角线上的值为dvalue或0，但实际并不用矩阵乘法实现

实现

```python
def backward(self, dvalue):
    # self.input和self.output形状是一样的
    # 那么dinput大小=doutput大小=dvalue大小
    # 可以用mask来更快实现，而不用矩阵运算
    self.dinput = dvalue.copy()
    self.dinput[self.input < 0] = 0
```

三、Categorical Cross-Entropy loss

公式

$$L_i = -\sum_j y_{i,j} log(\hat{y}_{i,j})$$

> 其中 L_i 表示样本损失值，i 表示集合中的第 i 个样本，j 表示标签索引，y 表示目标值，$\hat{y}$ 表示预测值。

$$\frac{\partial L_i}{\partial \hat{y}_{i,j}} = \frac{\partial}{\partial \hat{y}_{i,j}}[-\sum_j y_{i,j} log(\hat{y}_{i,j})] = -\sum_j y_{i,j} \cdot \frac{\partial}{\partial \hat{y}_{i,j}} log(\hat{y}_{i,j}) =$$

$$= -\sum_j y_{i,j} \cdot \frac{1}{\hat{y}_{i,j}} \cdot \frac{\partial}{\partial \hat{y}_{i,j}} \hat{y}_{i,j} = -\sum_j y_{i,j} \cdot \frac{1}{\hat{y}_{i,j}} \cdot 1 = -\sum_j \frac{y_{i,j}}{\hat{y}_{i,j}} = -\frac{y_{i,j}}{\hat{y}_{i,j}}$$

实现

```python
def backward(self, y_pred, y_true):
    n_sample = len(y_true)
    if len(y_true.shape) == 2:    # 标签是onehot的编码
        label = y_true
    elif len(y_true.shape) == 1:   # 只有一个类别标签
        # 将标签改成onehot的编码
        label = np.zeros((n_sample, len(y_pred[0])))
        label[range(n_sample), y_true] = 1
    self.dinput = - label / y_pred
    # 每个样本除以n_sample，因为在优化的过程中要对样本求和
    self.dinput = self.dinput / n_sample
```

四、Softmax

公式

Softmax函数是一种将j个实数向量转换为j个可能结果的概率分布的函数。索引i表示当前样本，索引j表示当前样本中的当前输出，$S_{i,j}$表示j个可能结果的概率。

$$S_{i,j} = \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}}$$

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \frac{\partial \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}}}{\partial z_{i,k}}$$

当$j = k$，推导如下：

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \frac{\partial \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}}}{\partial z_{i,k}} = \frac{\frac{\partial}{\partial z_{i,k}} e^{z_{i,j}} \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot \frac{\partial}{\partial z_{i,k}} \sum_{l=1}^{L} e^{z_{i,l}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} =$$

$$\frac{e^{z_{i,j}} \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} = \frac{e^{z_{i,j}} \cdot (\sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,k}})}{\sum_{l=1}^{L} e^{z_{i,l}} \cdot \sum_{l=1}^{L} e^{z_{i,l}}} =$$

$$\frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot \frac{\sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}} = \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot (\frac{\sum_{l=1}^{L} e^{z_{i,l}}}{\sum_{l=1}^{L} e^{z_{i,l}}} - \frac{e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}}) =$$

$$S_{i,j} \cdot (1 - S_{i,k})$$

当$j \neq k$，推导如下：

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \frac{\partial \frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}}}{\partial z_{i,k}} = \frac{\frac{\partial}{\partial z_{i,k}} e^{z_{i,j}} \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot \frac{\partial}{\partial z_{i,k}} \sum_{l=1}^{L} e^{z_{i,l}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} =$$

$$\frac{0 \cdot \sum_{l=1}^{L} e^{z_{i,l}} - e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} = \frac{-e^{z_{i,j}} \cdot e^{z_{i,k}}}{[\sum_{l=1}^{L} e^{z_{i,l}}]^2} = \frac{-e^{z_{i,j}} \cdot e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}} \cdot \sum_{l=1}^{L} e^{z_{i,l}}} =$$

$$-\frac{e^{z_{i,j}}}{\sum_{l=1}^{L} e^{z_{i,l}}} \cdot \frac{e^{z_{i,k}}}{\sum_{l=1}^{L} e^{z_{i,l}}} = -S_{i,j} \cdot S_{i,k}$$

综上有:

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \begin{cases} S_{i,j} \cdot (1 - S_{i,k}) & j = k \\ -S_{i,j} \cdot S_{i,k} & j \neq k \end{cases}$$

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = \begin{cases} S_{i,j} \cdot (1 - S_{i,k}) & j = k \\ S_{i,j} \cdot (0 - S_{i,k}) & j \neq k \end{cases}$$

$$\delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$\frac{\partial S_{i,j}}{\partial z_{i,k}} = S_{i,j} \cdot (\delta_{j,k} - S_{i,k}) = S_{i,j}\delta_{j,k} - S_{i,j}S_{i,k}$$

$$\frac{\partial loss}{\partial z_{i,k}} = \frac{\partial loss}{\partial S_{i,j}} \frac{\partial S_{i,j}}{\partial z_{i,k}}$$

实现

```python
def backward(self, dvalue):
    # input和output大小相同都为1xa，
    # loss是标量，那么dinput和doutput（即dvalue）大小相同都为1xa，
    # output对input的导数为一个axa的方阵

    # 相同大小的空矩阵
    self.dinput = np.empty_like(dvalue)
    # 对每个samlpe（每一行）循环
    for each, (single_output, single_dvalue) in enumerate(zip(self.output, dvalue)):
        # 显然这两种计算法算到的dinput大小是一样的
        # 这里是(1xa) * (axa) = 1xa是行向量
        self.dinput[each] = np.dot(single_dvalue,
                                   np.diagflat(single_output)-
np.dot(single_output.T, single_output))
        # 这里是(axa) * (1xa).T = ax1是个列向量
        # 但np默认会将列向量变为行向量，注意这里是列向量而不是列矩阵
        # self.dinput[each] = np.dot(
        #                                       np.diagflat(single_output) -
        #                                       np.dot(single_output.T, single_output),
        #                                       single_dvalue.T
        #                                       )
```

五、Sigmoid

公式

$$\sigma_{i,j} = \frac{1}{1 + e^{-z_{i,j}}}$$

其中$z_{i,j}$表示这个激活函数的输入，$\sigma_{i,j}$表示单个输出值。索引i表示当前样本，索引j表示当前样本中的当前输出。$\sigma_{i,j}$可理解成对第j对类别，例如猫狗分类中狗类别的confidence(置信度)。当然，一个模型可能要对多对类别分类，例如：高矮、胖瘦等。Sigmoid用于二分类

$$\sigma_{i,j} = \frac{1}{1+e^{-z_{i,j}}} \quad \rightarrow \quad \sigma'_{i,j} = \frac{d}{dz_{i,j}}\left[\frac{1}{1+e^{-z_{i,j}}}\right] = \frac{d}{dz_{i,j}}(1+e^{-z_{i,j}})^{-1} =$$

$$= -1\cdot(1+e^{-z_{i,j}})^{-1-1}\cdot\frac{d}{dz_{i,j}}(1+e^{-z_{i,j}}) = -(1+e^{-z_{i,j}})^{-2}\cdot\left(\frac{d}{dz_{i,j}}1+\frac{d}{dz_{i,j}}e^{-z_{i,j}}\right) =$$

$$= -(1+e^{-z_{i,j}})^{-2}\cdot\left(0+e^{-z_{i,j}}\cdot\frac{d}{dz_{i,j}}[-z_{i,j}]\right) =$$

$$= -(1+e^{-z_{i,j}})^{-2}\cdot\left(e^{-z_{i,j}}\cdot(-1\cdot\frac{d}{dz_{i,j}}z_{i,j})\right) = -(1+e^{-z_{i,j}})^{-2}\cdot(e^{-z_{i,j}}\cdot(-1)) =$$

$$= -(1+e^{-z_{i,j}})^{-2}\cdot(-e^{-z_{i,j}}) = (1+e^{-z_{i,j}})^{-2}\cdot e^{-z_{i,j}} =$$

$$= \frac{e^{-z_{i,j}}}{(1+e^{-z_{i,j}})^2} = \frac{e^{-z_{i,j}}}{(1+e^{-z_{i,j}})(1+e^{-z_{i,j}})} = \frac{1}{1+e^{-z_{i,j}}}\cdot\frac{e^{-z_{i,j}}}{1+e^{-z_{i,j}}} =$$

$$= \frac{1}{1+e^{-z_{i,j}}}\cdot\frac{1+e^{-z_{i,j}}-1}{1+e^{-z_{i,j}}} == \frac{1}{1+e^{-z_{i,j}}}\cdot\left(\frac{1+e^{-z_{i,j}}}{1+e^{-z_{i,j}}} - \frac{1}{1+e^{-z_{i,j}}}\right) =$$

$$= \frac{1}{1+e^{-z_{i,j}}}\cdot\left(1 - \frac{1}{1+e^{-z_{i,j}}}\right) = \sigma_{i,j}\cdot(1-\sigma_{i,j})$$

$$\frac{\partial loss}{\partial z_{i,k}} = \begin{cases} \frac{\partial loss}{\partial \sigma_{i,j}}\frac{\partial \sigma_{i,j}}{\partial z_{i,k}}, j=k \\ 0, j\neq k \end{cases}$$

k取一个固定值，那么j每取一个值，$\frac{\partial loss}{\partial z_{i,k}}$都是标量；而$\frac{\partial loss}{\partial z_{i,*}}$就是个行向量，$\frac{\partial \sigma_{i,*}}{\partial z_{i,*}}$是一个对角方阵。

这里可以用矩阵计算，但有更简单的方法，实现如下：

实现

```python
def backward(self, dvalue):
    # 这里也可以用矩阵计算，但dinput、dvalue、output大小相同，
    # 可以直接按元素对应相乘。
    self.dinput = dvalue * self.output * ( 1 - self.output )
```

六、Binary Cross-Entropy loss

公式

$$L_{i,j} = (y_{i,j})(-log(\hat{y}_{i,j})) + (1 - y_{i,j})(-log(1 - \hat{y}_{i,j})) =$$

$$= -y_{i,j} \cdot log(\hat{y}_{i,j}) - (1 - y_{i,j}) \cdot log(1 - \hat{y}_{i,j})$$

其中，j是第j对二进制输出。

$$\frac{\partial L_{i,j}}{\partial \hat{y}_{i,j}} = \frac{\partial}{\partial \hat{y}_{i,j}}[-y_{i,j} \cdot log(\hat{y}_{i,j}) - (1 - y_{i,j}) \cdot log(1 - \hat{y}_{i,j})] =$$

$$= \frac{\partial}{\partial \hat{y}_{i,j}}[-y_{i,j} \cdot log(\hat{y}_{i,j})] + \frac{\partial}{\partial \hat{y}_{i,j}}[-(1 - y_{i,j}) \cdot log(1 - \hat{y}_{i,j})] =$$

$$= -y_{i,j} \cdot \frac{\partial}{\partial \hat{y}_{i,j}}log(\hat{y}_{i,j}) - (1 - y_{i,j}) \cdot \frac{\partial}{\partial \hat{y}_{i,j}}log(1 - \hat{y}_{i,j}) =$$

$$= -y_{i,j} \cdot \frac{1}{\hat{y}_{i,j}} \cdot \frac{\partial}{\partial \hat{y}_{i,j}}\hat{y}_{i,j} - (1 - y_{i,j}) \cdot \frac{1}{1 - \hat{y}_{i,j}} \cdot \frac{\partial}{\partial \hat{y}_{i,j}}[1 - \hat{y}_{i,j}] =$$

$$= -y_{i,j} \cdot \frac{1}{\hat{y}_{i,j}} \cdot 1 - (1 - y_{i,j}) \cdot \frac{1}{1 - \hat{y}_{i,j}} \cdot (\frac{\partial}{\partial \hat{y}_{i,j}}1 - \frac{\partial}{\partial \hat{y}_{i,j}}\hat{y}_{i,j}) =$$

$$= -y_{i,j} \cdot \frac{1}{\hat{y}_{i,j}} \cdot 1 - (1 - y_{i,j}) \cdot \frac{1}{1 - \hat{y}_{i,j}} \cdot (0 - 1) =$$

$$= -\frac{y_{i,j}}{\hat{y}_{i,j}} + \frac{1 - y_{i,j}}{1 - \hat{y}_{i,j}} = -(\frac{y_{i,j}}{\hat{y}_{i,j}} - \frac{1 - y_{i,j}}{1 - \hat{y}_{i,j}})$$

实现

```python
def backward(self, y_pred, y_true):
    # 样本个数
    n_sample = len(y_true)
    # 注意：BinaryCrossentropy之前都是Sigmoid函数
    # Sigmoid函数很容易出现0和1的输出
    # 所以以1e-7为左边界
    # 另一个问题是将置信度向1移动，即使是非常小的值，
    # 为了防止偏移，右边界为1 - 1e-7
    y_pred = np.clip(y_pred, 1e-7, 1 - 1e-7)
    self.dinput = - y_true / y_pred + (1 - y_true) / (1 - y_pred)
    # 每个样本除以n_sample，因为在优化的过程中要对样本求和
    self.dinput = self.dinput / n_sample
```