

矩阵定义

$$X = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}, W = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix}, B = \begin{bmatrix} b_1 & b_2 \end{bmatrix}, Y = \begin{bmatrix} y_1 & y_2 \end{bmatrix}, Z = \begin{bmatrix} z_1 & z_2 \end{bmatrix}$$

前向传播 ¶

$$y_1 = x_1 * w_{11} + x_2 * w_{21} + x_3 * w_{31} + b_1$$

$$y_2 = x_1 * w_{12} + x_2 * w_{22} + x_3 * w_{32} + b_2$$

$$z_1 = \text{sigmoid}(y_1)$$

$$z_2 = \text{sigmoid}(y_2)$$

$$Y = X * W + B = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} * \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix} + \begin{bmatrix} b_1 & b_2 \end{bmatrix} = \begin{bmatrix} y_1 & y_2 \end{bmatrix}$$

$$Z = \text{sigmoid}(Y)$$

如果 Z 不是输出层，那么 Z 是下一层的输入(X)，而且如果 Z 是输出层，一般不激活(直接输出 Y)，或者理解为($Z = Y$)
用一个损失函数评价和标准值的距离，我们希望距离越小越好

$$\text{损失函数(MSE)} \quad \text{loss} = \sum_{i=1}^n \frac{(\text{out}_i - \text{label}_i)^2}{2}$$

可以理解为下面这个向量求和

$$\begin{bmatrix} \text{loss}_1 & \text{loss}_2 & \dots & \text{loss}_n \end{bmatrix} = \begin{bmatrix} \text{out}_1 - \text{label}_1 & \text{out}_2 - \text{label}_2 & \dots & \text{out}_n - \text{label}_n \end{bmatrix}$$

反向传播思路

目标求解每一层的 $\frac{\partial \text{loss}}{\partial w}$ 和 $\frac{\partial \text{loss}}{\partial b}$

$$\text{迭代 } w - lr * \frac{\partial \text{loss}}{\partial w} \quad \text{和} \quad b - lr * \frac{\partial \text{loss}}{\partial b}$$

达到减少 loss 的效果

$$\frac{\partial \text{loss}}{\partial w_{ij}} = \frac{\partial \text{loss}}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial w_{ij}}$$

$$\frac{\partial \text{loss}}{\partial b_j} = \frac{\partial \text{loss}}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial b_j}$$

$$\frac{\partial \text{loss}}{\partial z_j^{-1}} = \frac{\partial \text{loss}}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial z_j^{-1}}$$

z_j^{-1} 代表前一层的输出，即为这一层输入 x_j ，然后继续可以对前一层的误差进行求 w ， b ，和前前一层的误差

不激活时,可以看做 $z = y$ 那么 $\frac{\partial z_j}{\partial y_j} = 1$

反向传播中的标量形式

我们回顾一下, $loss = \sum_{i=1}^n \frac{(out_i - label_i)^2}{2} = \sum_{i=1}^n \frac{(z_i - label_i)^2}{2}$

$$\frac{\partial loss}{\partial z_j} = z_j - label_j$$

不激活的情况下 $\frac{\partial z_j}{\partial y_j} = 1$

用sigmoid激活的情况下 $\frac{\partial z_j}{\partial y_j} = (1 - \text{sigmoid}(y_j)) * \text{sigmoid}(y_j)$

这里说明一下函数 $f(x) = \text{sigmoid}(x)$ 的导数为 $\frac{\partial f(x)}{\partial x} = \text{sigmoid}(x) * (1 - \text{sigmoid}(x))$

这样(以sigmoid激活为例子) $\frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} = (z_j - label_j) * \text{sigmoid}(z_j) * (1 - \text{sigmoid}(z_j))$

weight 和 bias 标量形式推导

若计算 $\frac{\partial loss}{\partial w_{ij}} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial w_{ij}}$, 只需求 $\frac{\partial y_j}{\partial w_{ij}}$

若计算 $\frac{\partial loss}{\partial b_j} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial b_j}$, 只需求 $\frac{\partial y_j}{\partial b_j}$

以上面为例

$$y_1 = x_1 * w_{11} + x_2 * w_{21} + x_3 * w_{31} + b_1$$

得到一般的算式

$$y_j = x_1 * w_{1j} + x_2 * w_{2j} + \dots + x_i * w_{ij} + \dots + x_n * w_{nj} + b_j$$

我们可以一并得到

$$\frac{\partial y_j}{\partial w_{ij}} = x_i$$

$$\frac{\partial y_j}{\partial b_j} = 1$$

所以得出

$$\frac{\partial loss}{\partial w_{ij}} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial w_{ij}} = (z_j - label_j) * \text{sigmoid}(z_j) * (1 - \text{sigmoid}(z_j)) * x_i \quad [1]$$

$$\frac{\partial loss}{\partial b_j} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial b_j} = (z_j - label_j) * \text{sigmoid}(z_j) * (1 - \text{sigmoid}(z_j)) * 1 \quad [2]$$

前一层误差推导

这里推导 $\frac{\partial loss}{\partial z_j^{-1}} = \frac{\partial loss}{\partial x_j}$ 其中前一层的输出就是这一层的输入

$$loss = \sum_{i=1}^n \frac{(out_i - label_i)^2}{2} = \sum_{i=1}^n \frac{(z_i - label_i)^2}{2}$$

从刚才的正项传播:

$$y_1 = x_1 * w_{11} + x_2 * w_{21} + x_3 * w_{31} + b_1$$

$$y_2 = x_1 * w_{12} + x_2 * w_{22} + x_3 * w_{32} + b_2$$

可以发现 x_i 和 $y_j, j \in 1, 2, 3, \dots, n$ 有关, 就是和 y 中每一项有关

与上边 $weight$ 与 $bias$ 不同, $weight$ 和 $bias$ 仅与 y 中某一项有关

y 到 z 是单射函数, 所以 x_i 和 $z_j, j \in 1, 2, 3, \dots, n$ 有关,

如果计算 $\frac{\partial loss}{\partial z_j^{-1}} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial z_j^{-1}}$ 则需要计算 $\frac{\partial y_j}{\partial z_j^{-1}}$

求和

注意, 这里的 z_j^{-1} 就相当于这一层的 x_j

所以得到

$$\frac{\partial loss}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial x_j}$$

得到一般的算式

$$y_i = x_1 * w_{1i} + x_2 * w_{2i} + \dots + x_j * w_{ji} + \dots + x_m * w_{mi} + b_i$$

$$\frac{\partial y_i}{\partial z_j^{-1}} = w_{ji}$$

前一层误差推导

这里推导 $\frac{\partial loss}{\partial z_j^{-1}} = \frac{\partial loss}{\partial x_j}$ 其中前一层的输出就是这一层的输入

$$loss = \sum_{i=1}^n \frac{(out_i - label_i)^2}{2} = \sum_{i=1}^n \frac{(z_i - label_i)^2}{2}$$

从刚才的正项传播:

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可以发现 x_i 和 $y_j, j \in 1, 2, 3, \dots, n$ 有关, 就是和 y 中每一项有关

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y 到 z 是单射函数, 所以 x_i 和 $z_j, j \in 1, 2, 3, \dots, n$ 有关,

如果计算 $\frac{\partial loss}{\partial z_j^{-1}} = \frac{\partial loss}{\partial z_j} * \frac{\partial z_j}{\partial y_j} * \frac{\partial y_j}{\partial z_j^{-1}}$ 则需要计算 $\frac{\partial y_j}{\partial z_j^{-1}}$

求和

注意，这里的 z_j^{-1} 就相当于这一层的 x_j

所以得到

$$\frac{\partial loss}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial x_j}$$

得到一般的算式

$$y_i = x_1 * w_{1i} + x_2 * w_{2i} + \dots + x_j * w_{ji} + \dots + x_m * w_{mi} + b_i$$

$$\frac{\partial y_i}{\partial z_j^{-1}} = w_{ji}$$

$$\frac{\partial loss}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial z_j^{-1}} = \sum_{i=1}^n \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial y_i} * \frac{\partial y_i}{\partial x_j} = \sum_{i=1}^n (z_i - label_i) * sigmoid(z_i) * (1 - sigmoid(z_i)) * w_{ji}$$

矩阵形式的梯度

我们转换为矩阵形式，我们一开始定义的矩阵如下：

$$X = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}, W = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix}, B = \begin{bmatrix} b_1 & b_2 \end{bmatrix}, Y = \begin{bmatrix} y_1 & y_2 \end{bmatrix}, Z = \begin{bmatrix} z_1 & z_2 \end{bmatrix}$$

$$Y = XW + B$$

$$Z = sigmoid(Y)$$

$$\frac{\partial loss}{\partial Z} = Z - Label = \begin{bmatrix} z_1 - label_1 & z_2 - label_2 \end{bmatrix}$$

$$\frac{\partial z_j}{\partial y_j} = sigmoid(Y) * (1 - sigmoid(Y)) \quad * \text{为点乘(对应元素相乘)}$$

$$\frac{\partial loss}{\partial W} = X^T @ \frac{\partial loss}{\partial Z} * \frac{\partial Z}{\partial Y} * \frac{\partial Y}{\partial W} = (Z - Label) * sigmoid(Z) * (1 - sigmoid(Z)) \quad [4] \quad @ \text{为矩阵乘法}$$

$$\frac{\partial loss}{\partial B} = \frac{\partial loss}{\partial Z} * \frac{\partial Z}{\partial Y} * \frac{\partial Y}{\partial B} = (Z - Label) * sigmoid(Z) * (1 - sigmoid(Z)) \quad [5]$$

$$\frac{\partial loss}{\partial X} = \frac{\partial loss}{\partial Z} * \frac{\partial Z}{\partial Y} * \frac{\partial Y}{\partial X} = (Z - Label) * sigmoid(Z) * (1 - sigmoid(Z)) @ W^T \quad [6]$$

推导 [4] 的细节

[4]式是由 [1] 式得出

$$\text{不妨设 } A = \frac{\partial loss}{\partial Z} * \frac{\partial Z}{\partial Y} = (Z - Label) * sigmoid(Z) * (1 - sigmoid(Z))$$

由[1]可以得出

$$\begin{bmatrix} \frac{\partial loss}{\partial w_{11}} & \frac{\partial loss}{\partial w_{12}} & \dots & \frac{\partial loss}{\partial w_{1n}} \\ \frac{\partial loss}{\partial w_{21}} & \frac{\partial loss}{\partial w_{22}} & \dots & \frac{\partial loss}{\partial w_{2n}} \\ \dots & \dots & \dots & \dots \\ \frac{\partial loss}{\partial w_{m1}} & \frac{\partial loss}{\partial w_{m2}} & \dots & \frac{\partial loss}{\partial w_{mn}} \end{bmatrix} = \begin{bmatrix} x_1 * a_1 & x_1 * a_2 & \dots & x_1 * a_n \\ x_2 * a_1 & x_2 * a_2 & \dots & x_2 * a_n \\ \dots & \dots & \dots & \dots \\ x_m * a_1 & x_m * a_2 & \dots & x_m * a_n \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_m \end{bmatrix} \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix}$$

即为

$$\frac{\partial loss}{\partial W} = X^t @ A$$

[4]公式成立

推导 [6] 的细节

[6]式是由 [3] 式 得出

不妨设 $A = \frac{\partial loss}{\partial Z} * \frac{\partial Z}{\partial Y} = (Z - Label) * sigmoid(Z) * (1 - sigmoid(Z))$

$$\begin{aligned} \left[\begin{array}{cccc} \frac{\partial loss}{\partial x_1} & \frac{\partial loss}{\partial x_2} & \cdots & \frac{\partial loss}{\partial x_m} \end{array} \right] &= \left[\begin{array}{cccc} w_{11} * a_1 + w_{12} * a_2 + \cdots + x_{1n} * a_n & \cdots & w_{m1} * a_1 + w_{m2} * a_2 + \cdots + \end{array} \right] \\ &= \left[\begin{array}{cccc} a_1 & a_2 & \cdots & a_n \end{array} \right] \left[\begin{array}{cccc} w_{11} & w_{21} & \cdots & w_{m1} \\ w_{12} & w_{22} & \cdots & w_{m2} \\ \cdots & \cdots & \cdots & \cdots \\ w_{1n} & w_{2n} & \cdots & w_{mn} \end{array} \right] \end{aligned}$$

即为

$$\frac{\partial loss}{\partial X} = A @ W^T$$

[6]公式成立