

前向传播

$x: shape = (?, 784), y: shape = (?, 10), w: shape = (784, 10), b: shape = (10,)$

$z = xw + b$ shape(?, 10)

$$z_i = \sum_j x_j w_{ji} + b_i$$

$a = softmax(z): shape = (?, 10)$

$$a_i = softmax(z) = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

一个样本的损失: $loss = - \sum_i y_i \log a_i$, 其中 y_i 为真实值, 如果为第 i 个类别则为1, 否则为0。

损失函数对 z 求导:

$$\frac{\partial loss}{\partial z_i} = - \left(\frac{\partial (y_i * \log a_i)}{\partial a_i} \frac{\partial a_i}{\partial z_i} + \sum_{j \neq i} \frac{\partial (y_j * \log a_j)}{\partial a_j} \frac{\partial a_j}{\partial z_i} \right) \quad (1)$$

softmax函数对 z 求导:

$$\begin{aligned} \frac{\partial a_i}{\partial z_i} &= \frac{e^{z_i}}{\sum_j e^{z_j}} - \frac{e^{z_i}}{\sum_j e^{z_j}}^2 = a_i * (1 - a_i) \\ \frac{\partial a_i}{\partial z_j} &= - \frac{e^{z_i}}{\sum_j e^{z_j}}^2 * e^{z_j} = a_i * a_j, j \neq i \end{aligned} \quad (2)$$

将式2代入式1得:

$$\begin{aligned} \frac{\partial loss}{\partial z_i} &= - \left(\frac{y_i}{a_i} * a_i * (1 - a_i) + \sum_{j \neq i} \frac{y_j}{a_j} * a_i * a_j \right) \\ &= - (y_i - y_i * a_i + \sum_{j \neq i} y_j * a_i) = a_i - y_i \end{aligned}$$

对 w_{ji}, b_i 求导,

$$\begin{aligned} \frac{\partial loss}{\partial w_{ji}} &= \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial w_{ji}} = (a_i - y_i) * x_j \\ \frac{\partial loss}{\partial b_i} &= \frac{\partial loss}{\partial z_i} * \frac{\partial z_i}{\partial b_i} = (a_i - y_i) \end{aligned}$$

x 很大, z_i 可能值较大, 当 z_i 为100时, 造成softmax为 \inf/\inf , 导致 a_i 为nan x 归一化后, 将 w 初始化为很小的值, 这样避免 z_i 值过大。实际上, 当 i 不是真实类别是, a_i 趋向于0, 最终造成 \log 以0为底数, 此时loss会为nan