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Problem 1: Parial Derivative of the Softmax Regression

If we consider the softmax regression $y = \operatorname{softmax}(Wx + b)$ where $x \in R^d, b, y \in R^k$ Then we know that the cross entropy loss for a single sample is $J = -\sum_{k=1}^K t_k \log(y_k)$ where t_k denotes whether or not the sample is in the kth category.

denotes whether or not the sample is in the kth category. How can we derive the gradients $\frac{\partial J}{\partial w_{k,i}}$ and $\frac{\partial J}{\partial b_k}$

First, we recall the definition of the softmax function:

$$y_k = \frac{\exp(z_k)}{\sum_{j=1}^K \exp(z_j)}$$

where we set $z_k = w_k^{\top} x + b_k$. Now, recalling the chain rule, we can see that our partial derivatives can be computed as follows:

$$\begin{split} \frac{\partial J}{\partial w_{k,i}} &= \frac{\partial J}{\partial y_k} \frac{\partial y_k}{\partial z_k} \frac{\partial z_k}{\partial w_k} \\ \frac{\partial J}{\partial b_k} &= \frac{\partial J}{\partial y_k} \frac{\partial y_k}{\partial z_k} \frac{\partial z_k}{\partial b_k} \end{split}$$

Thus we proceed by finding $\frac{\partial J}{\partial z_k}$ as follows:

$$\begin{split} \frac{\partial J}{\partial z_k} &= \frac{\partial J}{\partial y_k} \frac{\partial y_k}{\partial z_k} \\ \frac{\partial J}{\partial y_k} &= \frac{\partial}{\partial y_k} t_k \log(y_k) \\ &= \frac{t_k}{y_k} \end{split}$$

generalizes across multiple elements

$$\begin{split} \frac{\partial y_k}{\partial z_k} &= \frac{\partial}{\partial z_k} \frac{\exp(z_k)}{\sum_{j=1}^K \exp(z_j)} \\ &= \frac{\frac{\partial}{\partial z_k} \exp(z_k) \cdot \left(\sum_{j=1}^K \exp(z_j)\right) - \exp(z_k) \cdot \frac{\partial}{\partial z_k} \left(\sum_{j=1}^K \exp(z_j)\right)}{\left(\sum_{j=1}^K \exp(z_j)\right)^2} \\ &= \frac{\exp(z_k) \cdot \sum_{j=1}^K \exp(z_k) - \exp(z_k) \exp(z_k)}{\left(\sum_{j=1}^K \exp(z_j)\right)^2} \\ &= \frac{\exp(z_k) \left(\sum_{j=1}^K \exp(z_j) - \exp(z_k)\right)}{\left(\sum_{j=1}^K \exp(z_j)\right)^2} \end{split}$$

$$=y_k(1-y_k) \qquad \text{since } y_k = \frac{\exp(z_k)}{\sum_{j=1}^K \exp(z_j)} \text{for } y_k, z_k = -y_k y_w \qquad \text{for } y_k, z_i$$

$$=y_k(\delta - y_i) = y_k - t_k$$

We can then easily find the derivative w.r.t. b and w:

$$\frac{\partial z}{\partial b} = 1 : \frac{\partial J}{\partial b_k} = y_k - t_k$$

$$\frac{\partial z}{\partial w} = x : \frac{\partial J}{\partial w_k} = x(y_k - t_k)$$

Problem 2: Partial Derivatives in Matrix form

Rewrite your solution to the above in matrix form.

We can rewrite both of these gradients in matrix form:

$$\frac{\partial J}{\partial b} = Y - \vec{y}$$
$$\frac{\partial J}{\partial w} = X^{\top} (Y - \vec{t})$$