

Cross-entropy & Kullback-Leibler Divergence

I. Prove that $\sum_i p(i) \log_2 \frac{p(i)}{q(i)} = H_q(p) - H(p)$, where $H_q(p)$ is the cross-entropy of q given the average distribution p , and $H(p)$ is the entropy of p .

$$\begin{aligned} H_q(p) - H(p) &= \sum_x p(x) \cdot \log \frac{1}{q(x)} - \sum_x p(x) \cdot \log \frac{1}{p(x)} = \\ &= \sum_x p(x) \cdot \left(\log \frac{1}{q(x)} - \log \frac{1}{p(x)} \right) = \sum_x p(x) \cdot \log \frac{p(x)}{q(x)}. \end{aligned}$$

II. Neural network returns an output vector: $[-1, 2, 0]$. Use an appropriate function (softmax, sigmoid) for the classification task to produce a vector on which we can use cross-entropy loss measure.

a) Multi-class problem.

$$\left[\frac{e^{-1}}{e^{-1} + e^2 + e^0}; \frac{e^2}{e^{-1} + e^2 + e^0}; \frac{e^0}{e^{-1} + e^2 + e^0} \right] = [0.042; 0.844; 0.114].$$

b) Multi-label problem.

$$\left[\frac{e^{-1}}{1 + e^{-1}}; \frac{e^2}{1 + e^2}; \frac{e^0}{1 + e^0} \right] = [0.268; 0.88; 0.5].$$

III. Use the values above to compute a cross-entropy loss, if a correct output vector for this particular case was $[0, 1, 0]$. Take into account the type of classification problem, so that the error makes sense.

a) Multi-class problem.

$$\begin{aligned} & \text{from II a) } [-1; 2; 0] \rightarrow [0.042; 0.844; 0.114] \\ & t = [0, 1, 0]; \\ & y = [0.042; 0.844; 0.114] \end{aligned} \quad \left. \vphantom{\begin{aligned} & \text{from II a) } [-1; 2; 0] \rightarrow [0.042; 0.844; 0.114] \\ & t = [0, 1, 0]; \\ & y = [0.042; 0.844; 0.114] \end{aligned}} \right\} CE(t, y) = 0 \cdot \log \frac{1}{0.042} + 1 \cdot \log \frac{1}{0.844} + 0 \cdot \log \frac{1}{0.114} = \log \frac{1}{0.844} = 0.17.$$

b) Multi-label problem.

$$\begin{aligned}
 & \text{from IIb) } [-1, 2, 0] \rightarrow [0.268, 0.88, 0.5]. \\
 & t = [0, 1, 0]; \\
 & y = [0.268, 0.88, 0.5] \quad \left\{ \begin{aligned} CE(t, y) &= CE_1 + CE_2 + CE_3 = 0 \cdot \log \frac{1}{1-0.268} + \\ &+ 1 \cdot \log \frac{1}{0.268} + 1 \cdot \log \frac{1}{0.88} + 0 \cdot \log \frac{1}{1-0.88} + 0 \cdot \log \frac{1}{1-0.5} + \\ &+ 1 \cdot \log \frac{1}{0.5} = \log \frac{1}{0.268} + \log \frac{1}{0.88} + \log \frac{1}{0.5} = 1.32 + 0.69 + \\ &+ 0.13 = 2.01 + 0.13 = 2.14. \end{aligned} \right.
 \end{aligned}$$

IV. Compute a Kullback-Leibler divergence (relative entropy) between the probability distributions. Compare the result when distributions are swapped.

a) $P_1 = \{0.5, 0.5\}$, $P_2 = \{0.25, 0.75\}$: $d_{KL}(P_1 \parallel P_2)$ and $d_{KL}(P_2 \parallel P_1)$

$$\begin{aligned}
 1) d_{KL}(P_1 \parallel P_2) &= 0.5 \cdot \log \frac{1}{0.25} + 0.5 \cdot \log \frac{1}{0.75} - 0.5 \cdot \log \frac{1}{0.5} - \\
 &- 0.5 \cdot \log \frac{1}{0.5} = 0.5 \cdot (1.386 + 0.287 - 0.69 - 0.69) = \\
 &= 0.1375. \\
 2) d_{KL}(P_2 \parallel P_1) &= 0.25 \cdot \log \frac{1}{0.5} + 0.75 \cdot \log \frac{1}{0.5} - 0.25 \cdot \log \frac{1}{0.25} - \\
 &- 0.75 \cdot \log \frac{1}{0.75} = 0.25 \cdot (0.69 - 1.386) + 0.75 \cdot (0.69 - 0.287) \\
 &= -0.174 + 0.3075 = 0.1335. \\
 d_{KL}(P_1 \parallel P_2) &= 0.1375 > d_{KL}(P_2 \parallel P_1) = 0.1335.
 \end{aligned}$$

b) $P_1 = \{0.25, 0.25, 0.5\}$, $P_2 = \{0.1, 0.2, 0.7\}$: $d_{KL}(P_1 \parallel P_2)$ and $d_{KL}(P_2 \parallel P_1)$

$$\begin{aligned}
 1) d_{KL}(P_1 \parallel P_2) &= 0.25 \cdot \log \frac{1}{0.1} + 0.25 \cdot \log \frac{1}{0.2} + 0.5 \cdot \log \frac{1}{0.7} - \\
 &- 0.25 \cdot \log \frac{1}{0.25} - 0.25 \cdot \log \frac{1}{0.25} - 0.5 \cdot \log \frac{1}{0.5} = 0.25 \cdot (2.3 + 1.6 - \\
 &- 1.386 - 1.386) + 0.5 \cdot (0.356 - 0.69) = 0.115. \\
 2) d_{KL}(P_2 \parallel P_1) &= 0.1 \cdot \log \frac{1}{0.25} + 0.2 \cdot \log \frac{1}{0.25} + 0.7 \cdot \log \frac{1}{0.5} - \\
 &- 0.1 \cdot \log \frac{1}{0.1} - 0.2 \cdot \log \frac{1}{0.2} - 0.7 \cdot \log \frac{1}{0.7} = 0.1 \cdot (1.386 - \\
 &- 2.3) + 0.2 \cdot (1.386 - 1.6) + 0.7 \cdot (0.69 - 0.356) = 0.0996. \\
 d_{KL}(P_1 \parallel P_2) &= 0.115 > d_{KL}(P_2 \parallel P_1) = 0.0996.
 \end{aligned}$$

$$\begin{aligned}
 d_{KL}(p \parallel q) &= H(p \parallel q) - H(p) = E_p \left(\log \frac{1}{q} \right) - E_p \left(\log \frac{1}{p} \right) = \\
 &= \sum_x p(x) \cdot \log \frac{1}{q(x)} - \sum_x p(x) \cdot \log \frac{1}{p(x)}.
 \end{aligned}$$