

Suppose there are an arbitrary input  $x \in \mathbb{R}^2$  and an arbitrary output  $y \in \{0, 1\}$ , and their probabilistic assumption is given by

$$p(\theta, x, y) = p(\theta)p(x)p(y|x; \theta), \quad (1)$$

where  $q_\theta(x) := p(1|x; \theta)$  is modeled by the neural classifier with parameter  $\theta$ . Also, assume a dataset  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$  of  $N$  data points is given. Our goal is to make the Bayesian classifier for this dataset. Specifically, we want to learn

$$p(y|x) = \int p(y|x; \theta)p(\theta|\mathcal{D})d\theta \approx \frac{1}{N} \sum_{i=0}^{N-1} p(y|x; \theta_i), \quad (2)$$

where  $\theta_0, \dots, \theta_{N-1}$  are sampled from the posterior distribution  $p(\theta|\mathcal{D})$  by Stein variational gradient descent (SVGD). From model assumption, we can say

$$p(\theta, \mathcal{D}) = p(\theta)p(\mathcal{D}|\theta) = p(\theta) \prod_{i=0}^{N-1} p(x_i)p(y_i|x_i; \theta) \quad (3)$$

$$= p(\theta) \prod_{i=0}^{N-1} p(x_i)q_\theta(x_i)^{y_i}(1 - q_\theta(x_i))^{1-y_i}, \quad (4)$$

and the log posterior is

$$\log p(\theta|\mathcal{D}) = \log p(\theta) + \sum_{i=0}^{N-1} \{\log p(x_i) + y_i \log q_\theta(x_i) + (1 - y_i) \log(1 - q_\theta(x_i))\} - \log p(\mathcal{D}). \quad (5)$$

If we assume uniform prior  $p(\theta)$  and ignore the terms that will not affect the gradient w.r.t.  $\theta$ , the log posterior becomes

$$\log p(\theta|\mathcal{D}) = \sum_{i=0}^{N-1} \{y_i \log q_\theta(x_i) + (1 - y_i) \log(1 - q_\theta(x_i))\} + \text{constant} \quad (6)$$

Note that the term in summation is the same as the negative cross entropy which enables us to use cross entropy implementation in TensorFlow.