## Homework Assignment 5

Lecturer: Kyunghyun Cho

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1. The probability density function of normal distribution is defined as

$$f(\mathbf{x}) = \frac{1}{Z} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\top} \boldsymbol{\Sigma}^{-1}(\mathbf{s} - \boldsymbol{\mu})\right),$$

where

$$Z = \int_{\mathbf{x} \in \mathbb{R}^d} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\top} \boldsymbol{\Sigma}^{-1}(\mathbf{s} - \boldsymbol{\mu})\right) d\mathbf{x}$$
$$= (2\pi)^{-d/2} |\boldsymbol{\Sigma}|^{-1/2},$$

where  $|\Sigma|$  is the determinant of the covariance matrix.

Let us assume that the covariance matrix  $\Sigma$  is a diagonal matrix, as below:

$$\Sigma = \left[ egin{array}{cccc} oldsymbol{\sigma}_1^2 & 0 & \cdots & 0 \ 0 & oldsymbol{\sigma}_2^2 & \cdots & 0 \ dots & 0 & \cdots & 0 \ dots & dots & \cdots & dots \ 0 & 0 & \cdots & oldsymbol{\sigma}_d^2 \ \end{array} 
ight].$$

The probability density function simplifies to

$$f(\mathbf{x}) = \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{1}{2} \frac{1}{\sigma_i^2} (x_i - \mu_i)^2\right).$$

Show that this is indeed true.

2.

(a) Show that the following equation, called Bayes' rule, is true.

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}.$$

(b) We learned the definition of expectation:

$$\mathbb{E}[X] = \sum_{x \in \Omega} x p(x).$$

Assuming that X and Y are discrete random variables, show that

$$\mathbb{E}\left[X+Y\right] = \mathbb{E}\left[X\right] + \mathbb{E}\left[Y\right].$$

(c) Further assume that  $c \in \mathbb{R}$  is a scalar and is not a random variable, show that

$$\mathbb{E}\left[cX\right] = c\mathbb{E}\left[X\right].$$

(d) We learned the definition of variance:

$$\operatorname{Var}(X) = \sum_{x \in \Omega} (x - \mathbb{E}[X])^2 p(x).$$

Assuming X being a discrete random variable, show that

$$\operatorname{Var}(X) = \mathbb{E}\left[X^2\right] - \left(\mathbb{E}\left[X\right]\right)^2.$$

**3.** An optimal linear regression machine (without any regularization term), that minimizes the empirical cost function given a training set

$$D_{\text{tra}} = \{(\mathbf{x}_1, \mathbf{y}_1^*), \dots, (\mathbf{x}_N, \mathbf{y}_N^*)\},\$$

can be found directly without any gradient-based optimization algorithm. Assuming that the distance function is defined as

$$D(M^*(\mathbf{x}), M, \mathbf{x}) = \frac{1}{2} \|M^*(\mathbf{x}) - M(\mathbf{x})\|_2^2 = \frac{1}{2} \sum_{k=1}^q (y_k^* - y_k)^2,$$

derive the optimal weight matrix W. (Hint: Moore–Penrose pseudoinverse)

**4.** Suppose that we have a data distribution  $Y = f(\mathbf{X}) + \varepsilon$ , where **X** is a random vector,  $\varepsilon$  is an independent random variable with zero mean and fixed but unknown variance  $\sigma^2$ , and f is an unknown deterministic function that maps a vector into a scalar.

Now, we wish to approximate  $f(\mathbf{x})$  with our own model  $\hat{f}(\mathbf{x}; \Theta)$  with some learnable parameters  $\Theta$ .

(a) Show that considering all possible  $\hat{f}$  and  $\Theta$ , the minimum of L2 loss

$$\mathbb{E}_{\mathbf{X}}[(Y - \hat{f}(\mathbf{X}; \mathbf{\Theta}))^2]$$

is achieved when for all x,

$$\hat{f}(\mathbf{x}; \mathbf{\Theta}) = f(\mathbf{x})$$

(Hint: find the minimum of L2 loss for a single example first.)

(b) If we train the same model varying initializations and examples from the underlying data distribution, we may end up with different  $\Theta$ . So we can also consider  $\Theta$  as a random variable if we fix  $\hat{f}$ .

Show that for a single unseen input vector  $\mathbf{x}_0$  and a fixed  $\hat{f}$ , the expected squared error between the ground truth  $f(\mathbf{x}_0)$  and the prediction  $\hat{f}(\mathbf{x}_0; \Theta)$  can be decomposed into:

$$\mathbb{E}[(f(\mathbf{x}_0) - \hat{f}(\mathbf{x}_0; \Theta))^2] = (\mathbb{E}[f(\mathbf{x}_0) - \hat{f}(\mathbf{x}_0; \Theta)])^2 + \operatorname{Var}[\hat{f}(\mathbf{x}_0; \Theta)] + \sigma^2$$

(Side note: this is usually known as the *bias-variance decomposition*, closely related to *bias-variance tradeoff*, and other concepts such as underfitting and overfitting.)