Introduction to Machine Learning, Spring 2022

Homework 1

(Due Friday, Mar. 18 at 11:59pm (CST))

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1. [10 points] Given the input variables $X \in \mathbb{R}^p$ and output variable $Y \in \mathbb{R}$, the Expected Prediction Error (EPE) is defined by

$$EPE(\hat{f}) = \mathbb{E}[L(Y, f(X))], \tag{1}$$

where $\mathbb{E}(\cdot)$ denotes the expectation over the joint distribution $\Pr(X,Y)$, and L(Y,f(X)) is a loss function measuring the difference between the estimated f(X) and observed Y. We have shown in our course that for the squared error loss $L(Y,f(X))=(Y-f(X))^2$, the regression function $f(x)=\mathbb{E}(Y|X=x)$ is the optimal solution of $\min_f \operatorname{EPE}(f)$ in the pointwise manner.

(a) In Least Squares, a linear model $X^{\top}\beta$ is used to approximate f(X) according to

$$\min_{\beta} \mathbb{E}[(Y - X^{\top}\beta)^2]. \tag{2}$$

Please derive the optimal solution of the model parameters β . [3 points]

- (b) Please explain how the nearest neighbors and least squares approximate the regression function, and discuss their difference. [3 points]
- (c) Given absolute error loss L(Y, f(X)) = |Y f(X)|, please prove that f(x) = median(Y|X = x) minimizes EPE(f) w.r.t. f. [4 points]

Solution:

(a)

$$\frac{\partial E[(Y - X^T \beta)^2]}{\partial \beta} = -2X^T (Y - X^T \beta) E[(Y - X^T \beta)]$$

Let

$$\frac{\partial E[(Y - X^T \beta)^2]}{\partial \beta} = 0$$

 $E[(Y - X^T \beta)^2] > 0, X^T$ is a $1 \times p$ matrix, so

$$Y - X^T \beta = 0$$

Thus,

$$\beta = (X^T)^{-1}Y$$

- (b) The nearest neighbors: $\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$ Firstly, it uses the neighbours information to approximate the current point. Also, it uses the average value instead of the approximate expectation. The least squares:
- (c)

2. [10 points] Consider real-valued variables X and Y, in which Y is generated conditional on X according to

$$Y = aX + b + \epsilon$$
, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

Here ϵ is an independent variable, called a noise term, which is drawn from a Gaussian distribution with mean 0, and variance σ^2 . This is a single variable linear regression model, where a is the only weight parameter and b denotes the intercept. The conditional probability of Y has a distribution $p(Y|X,a,b) \sim \mathcal{N}(aX+b,\sigma^2)$, so it can be written as:

$$p(Y|X,a,b) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(Y - aX - b)^2\right).$$

- (a) Assume we have a training dataset of n i.i.d. pairs (x_i, y_i) , i = 1, 2, ..., n, and the likelihood function is defined by $L(a, b) = \prod_{i=1}^{n} p(y_i|x_i, a, b)$. Please write the Maximum Likelihood Estimation (MLE) problem for estimating a and b. [3 points]
- (b) Estimate the optimal solution of a and b by solving the MLE problem in (a). [4 points]
- (c) Based on the result in (b), argue that the learned linear model f(X) = aX + b, always passes through the point (\bar{x}, \bar{y}) , where $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ and $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$ denote the sample means. [3 points]

3. [10 points] Given a set of training data $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$ from which to estimate the parameters $\boldsymbol{\beta}$, where each $\mathbf{x}_i = [x_{i1}, \dots, x_{ip}]^T$ denotes a vector of feature measurements for the *i*th sample. Consider a linear regression problem in which we want to "weight" different training examples differently. Specifically, suppose we aim at minimizing

$$RSS(\boldsymbol{\beta}) = \frac{1}{2} \sum_{i=1}^{N} w_i (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2.$$
 (3)

- (a) Show that $RSS(\boldsymbol{\beta}) = (\mathbf{X}\boldsymbol{\beta} \mathbf{y})^T \mathbf{W} (\mathbf{X}\boldsymbol{\beta} \mathbf{y})$ for an appropriate diagonal matrix \mathbf{W} , and where $\mathbf{X} = [\mathbf{x}_1, \cdots, \mathbf{x}_N]^T$ and $\mathbf{y} = [y_1, \cdots, y_N]^T$. Please state clearly what \mathbf{W} is. [2 points]
- (b) By finding the derivative $\nabla_{\beta} RSS(\beta)$ w.r.t. β and setting that to zero, derive the closed-form solution of β that minimizes $RSS(\beta)$. [3 points]
- (c) Is there any way to control the model complexity in (3)? If yes, please formulate the $RSS(\beta)$ and estimate its closed-form solution of β . [5 points]