Exercises for the course

Machine Learning 1

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Exercise Sheet 7

Exercise 1: Bias and Variance of Mean Estimators (20 P)

Assume we have an estimator $\hat{\theta}$ for a parameter θ. The bias of the estimator $\hat{\theta}$ is the difference between the true value for the estimator, and its expected value:

$$\mathrm{Bias}(\hat{\theta}) = \mathrm{E}\big[\hat{\theta} - \theta\big].$$

If $\mathrm{Bias}(\hat{\theta}) = 0$, then $\hat{\theta}$ is called unbiased. The variance of the estimator $\hat{\theta}$ is the expected square deviation from its expected value:

$$\mathrm{Var}(\hat{\theta}) = \mathrm{E}\big[(\hat{\theta} - \mathrm{E}[\hat{\theta}])^2\big].$$

The mean squared error of the estimator $\hat{\theta}$ is

$$\mathrm{Error}(\hat{\theta}) = \mathrm{E}\big[(\hat{\theta} - \theta)^2\big] = \mathrm{Bias}(\hat{\theta})^2 + \mathrm{Var}(\hat{\theta})$$

Let $X_1, \dots, X_N$ be a sample of i.i.d random variables. Assume that X_i has mean μ and variance σ^2. *Calculate* the bias, variance and mean squared error of the following mean estimators:

(a) $\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} X_i$ (i.e. the sample mean),

(b) $\hat{\mu} = 0$.

Exercise 2: Bias-Variance Decomposition for Regression (15 P)

Let $y = f(x)$ be a function mapping input to output and evaluated at some out-of-sample data point x. Consider an estimator $\hat{f}(x)$ that is obtained by training a regression model on some random sample $\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\}$ of the function $y = f(x)$.

(a) *Prove* the bias-variance decomposition

$$\mathrm{Error}(\hat{f}(x)) = \mathrm{Bias}(\hat{f}(x))^2 + \mathrm{Var}(\hat{f}(x))$$

where the mean squared error, bias and variance are given by

$$\mathrm{Error}(\hat{f}(x)) = \mathrm{E}\big[(\hat{f}(x) - f(x))^2\big], \qquad \mathrm{Bias}(\hat{f}(x)) = \mathrm{E}\big[\hat{f}(x) - f(x)\big], \qquad \mathrm{Var}(\hat{f}(x)) = \mathrm{E}\big[(\hat{f}(x) - \mathrm{E}[\hat{f}(x)])^2\big].$$

Exercise 3: Bias-Variance Decomposition for Classification (15 P)

The bias-variance decomposition usually applies to regression data. In this exercise, we would like to obtain similar decomposition for classification, in particular, when the prediction is given as a probability distribution over C classes. Let $P = [P_1, \dots, P_C]$ be the ground truth class distribution associated to a particular input pattern. Assume a random estimator of class probabilities $\hat{P} = [\hat{P}_1, \dots, \hat{P}_C]$ for the same input pattern. The error function is given by the KL-divergence between the ground truth and the estimated probability distribution:

$$\mathrm{Error} = \mathrm{E}\big[D_{\mathrm{KL}}(P||\hat{P})\big].$$

First, we would like to determine the mean of of the class distribution estimator $\hat{P}$. We define the mean as the distribution that minimizes its expected KL divergence from the the class distribution estimator, that is, the distribution R that optimizes

$$\min_R \; \mathrm{E}\big[D_{\mathrm{KL}}(R||\hat{P})\big].$$

(a) *Show* that the solution to the optimization problem above is given by

$$R = [R_1, \dots, R_C] \quad \text{where} \quad R_i = \frac{\exp \mathrm{E}\big[\log \hat{P}_i\big]}{\sum_j \exp \mathrm{E}\big[\log \hat{P}_j\big]} \qquad \forall\, 1 \leq i \leq C.$$

(b) *Prove* the bias-variance decomposition

$$\mathrm{Error}(\hat{P}) = \mathrm{Bias}(\hat{P}) + \mathrm{Var}(\hat{P})$$

where the error, bias and variance are given by

$$\mathrm{Error}(\hat{P}) = \mathrm{E}\big[D_{\mathrm{KL}}(P||\hat{P})\big], \qquad \mathrm{Bias}(\hat{P}) = D_{\mathrm{KL}}(P||R), \qquad \mathrm{Var}(\hat{P}) = \mathrm{E}\big[D_{\mathrm{KL}}(R||\hat{P})\big].$$

Exercise 4: Programming (50 P)

Download the programming files on ISIS and follow the instructions.