Homework 2. Machine Learning (MIIS)

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Consider a simplified learning scenario. Assume that the input dimension is one. Assume that the input variable x is uniformly distributed in the interval [-1, 1]. The data set consists of 2 points $\{x_1, x_2\}$ and assume that the target function is $f(x) = x^2$. Thus, the full data set is $D = \{(x_1, x_1^2), (x_2, x_2^2)\}$. The learning algorithm returns the line fitting these two points as g (H consists of functions of the form $h(x) = ax + b$). We are interested in the test performance (E_{out}) of our learning system with respect to the squared error measure, the bias and the variance.

(a) Give the analytic expression for the average function $\bar{g}(x)$.

Hypothesis $g^D(x)$, where $D = \{(x_1, x_1^2), (x_2, x_2^2)\}$:

$$g^{\mathrm{D}}(x) = \left(\frac{{x_2}^2 - {x_1}^2}{x_2 - x_1}\right)(x - x_1) + {x_1}^2 \tag{1}$$

Which leads to:

$$g^{\mathrm{D}}(x) = (x_1 + x_2)x - x_1 x_2 \tag{2}$$

$\bar{g}(x)$ is defined as:

$$\bar{g}(x) = E_{\mathrm{D}}[g^{\mathrm{D}}(x)] \tag{3}$$

Then, computing the expectation for all the possible datasets:

$$\bar{g}(x) = \frac{1}{2}\int_{-1}^{1}\frac{1}{2}\int_{-1}^{1} g^{\mathrm{D}}(x)\,dx_1\,dx_2 = \frac{1}{4}\int_{-1}^{1}\int_{-1}^{1}(x_1+x_2)x - x_1x_2\,dx_1\,dx_2 = \frac{1}{4}\int_{-1}^{1} 2x_1x\,dx_1 = 0 \tag{4}$$

(b) Describe an experiment that you could run to determine (numerically) $\bar{g}(x)$, E_{out}, bias, and var.

We could determine experimentally these parameters by running a large amount of linear regression trainings. In each iteration, we would:

(a) Generate a dataset $D = \{(x_1, x_1^2), (x_2, x_2^2)\}$ with random x_1 and x_2 and a large dataset $D_{val} = \{(x_1, x_1^2) \ldots (x_N, x_N^2)\}$.

(b) Train $g^D(x)$

(c) Compute the error of $g^D(x)$ with D_{val}.

After all the iterations are finished, we can obtain E_{out} by taking the mean for all the linear regression errors.
$\bar{g}(x)$ can be obtained by computing the mean of all the weights for each $g^D(x)$.
Bias can be obtained by computing the error of $\bar{g}(x)$.
Variance can be computed taking the squared difference between the output of each $g^D(x)$ and $\bar{g}(x)$.

(c) Run your experiment and report the results. Compare E_{out} with bias+var. Provide a plot of your $\bar{g}$(x) and f(x) (on the same plot).

For the experiments, I computed 10.000 g^D(x) and generated a D_{val} of 1.000 samples for each iteration. The results are the following:

$E_{out} = 0.5341$
$bias = 0.2027$
$variance = 0.3356$
$bias + variance = 0.5384$

As expected, $E_{out} \approx bias + variance$

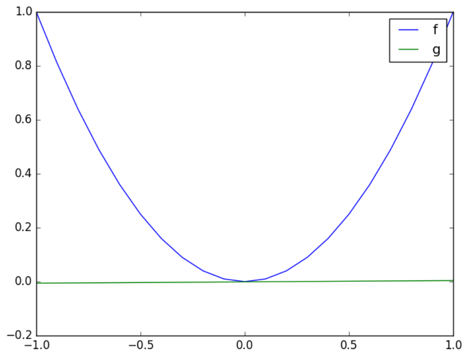

Figure 1: Comparison between $f(x)$ and $\bar{g}$(x).

(d) Compute analytically what E_{out}, bias, and var should be.

E_{out}:

$$E_{out} = E_D[E_{out}(g^D)] = E_D[E_x[(g^D(x) - f(x))^2]] \tag{5}$$

Combining (2), (5) and $f(x) = x^2$, we get:

$$E_{out} = \frac{1}{8}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}(g^D(x) - f(x))^2\,dx\,dx_1\,dx_2 = \frac{8}{15} \approx 0.5333$$

bias:

$$bias = E_x[(\bar{g}(x) - f(x))^2] = E_x[(\bar{g}(x) - f(x))^2] \tag{6}$$

Knowing (4) and $f(x) = x^2$:

$$bias = E_x[f(x)^2] = \frac{1}{2}\int_{-1}^{1} x^4\,dx = \frac{1}{5} \approx 0.2$$

variance:

$$variance = E_x[E_D[(g^D(x) - \bar{g}(x))^2]] \tag{7}$$

Knowing (2) and (4):

$$variance = E_{\mathrm{x}}[E_{\mathrm{D}}[g^{\mathrm{D}}(x)^2]] = \frac{1}{8}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}((x_1+x_2)x - x_1x_2)^2\, dx\, dx_1\, dx_2 = \frac{1}{3} \approx 0.333$$

As we can see, the results are almost identical to the ones obtained in the experiment. The small differences can be blamed to the fact that, as we can see in Figure 1, the experimental $\bar{g}$(x) is not 0 (as computed analytically), but has a small slope and a small bias.