

ECE 2372 - Homework 5
<< — Bias-Variance Decomposition — >>

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Problem 1:

Consider a learning scenario where $x \in \mathbb{R}$ and $y \in \mathbb{R}$ is given by $y = x^2$.

Assume that the input variable x is drawn uniformly on the interval $[-1, 1]$ and we are given two independent observations $\mathcal{D} = \{(x_1, y_1), (x_2, y_2)\}$.

We'll consider two different approaches to fitting a line to this data set, and we will be interested in calculating the expected risk (in terms of squared error), the bias, and the variance.

(a) Suppose $h(x) = b$, i.e., constant line. We are considering here to fit the line by setting

$$\begin{aligned} h_{\mathcal{D}}(x) &= \frac{y_1 + y_2}{2} \\ &= \frac{x_1^2 + x_2^2}{2} \end{aligned}$$

Derive (analytically) the average hypothesis: $\bar{h}(x) = \mathbb{E}_{\mathcal{D}} [h_{\mathcal{D}}(x)]$

a)

$$\bar{h}(x) = E_{\mathcal{D}}[h_{\mathcal{D}}(x)] = E_{\mathcal{D}}\left[\frac{x_1^2 + x_2^2}{2}\right] = \frac{1}{2}E_{\mathcal{D}}[x_1^2] + \frac{1}{2}E_{\mathcal{D}}[x_2^2]$$

Calculate the expectation $E[x^2]$:

$$E_{\mathcal{D}}[x^2] = \int_{-1}^1 p(x) * x^2 dx$$

The x is drawn uniformly on the interval $[-1, 1]$, therefore

$$p(x) = \frac{1}{2}$$

$$E_{\mathcal{D}}[x^2] = \int_{-1}^1 \frac{1}{2} * x^2 dx = \frac{1}{2} * \frac{x^3}{3} \Big|_{-1}^1 = \frac{1}{3}$$

Substitute to the equation:

$$\bar{h}(x) = \frac{1}{2} * \frac{1}{3} + \frac{1}{2} * \frac{1}{3} = \frac{1}{3}$$

(b) Compute (analytically) the bias

$$\mathbb{E}_X [(\bar{h}(X) - X^2)^2]$$

b)

$$\begin{aligned} E_x [(\bar{h}(x) - x^2)^2] &= E_x \left[\left(\frac{1}{3} - x^2 \right)^2 \right] = E_x \left[\frac{1}{9} - \frac{2}{3}x^2 + x^4 \right] \\ &= \frac{1}{9} - \frac{2}{3}E_x[x^2] + E_x[x^4] \end{aligned}$$

Calculate the expectation $E[x^4]$:

$$E_x[x^4] = \int_{-1}^1 p(x) * x^4 dx = \int_{-1}^1 \frac{1}{2} * x^4 dx$$

$$= \frac{1}{2} * \frac{x^5}{5} \Big|_{-1}^1 = \frac{1}{5}$$

Substitute to the equation:

$$Bias = E_x \left[(\bar{h}(x) - x^2)^2 \right] = \frac{1}{9} - \frac{2}{3} * \frac{1}{3} + \frac{1}{5} = \frac{4}{45}$$

(c) Compute (analytically) the variance

$$\mathbb{E}_X \left[E_{\mathbb{D}} \left[(h_{\mathbb{D}}(X) - \bar{h}(X))^2 \right] \right]$$

c)

$$E_x \left[E_{\mathbb{D}} \left[(h_{\mathbb{D}}(x) - \bar{h}(x))^2 \right] \right] = E_x \left[E_{\mathbb{D}} \left[\left(\frac{x_1^2 + x_2^2}{2} - \frac{1}{3} \right)^2 \right] \right] = E_x \left[E_{\mathbb{D}} \left[\frac{1}{9} - \frac{x_1^2 + x_2^2}{3} + \frac{x_1^4 + 2x_1^2x_2^2 + x_2^4}{4} \right] \right]$$

Calculate the expectation $E[x_1^2x_2^2]$:

$$E_{\mathbb{D}}[x_1^2x_2^2] = \int_{-1}^1 \int_{-1}^1 p(x_1)p(x_2) * x_1^2x_2^2 dx_1dx_2 = \frac{1}{3} * \frac{1}{3} = \frac{1}{9}$$

Substitute to the equation:

$$Variance = E_x \left[\frac{1}{9} - \frac{\left(\frac{1}{3} + \frac{1}{3}\right)}{3} + \frac{\frac{1}{5} + 2 * \frac{1}{9} + \frac{1}{5}}{4} \right] = E_x \left[\frac{1}{9} - \frac{2}{9} + \frac{7}{45} \right] = E_x \left[\frac{2}{45} \right] = \int_{-1}^1 \frac{1}{2} * \frac{2}{45} dx = \frac{2}{45}$$

(d) Now simulate this. Explicitly, numerically estimate average hypothesis, the bias, the variance and $\bar{h}(x) = \mathbb{E}_{\mathbb{D}} [R(h_{\mathbb{D}})]$

The code is in HW5_1_d .

From interval $[-1,1]$, drawn 10000 data set uniformly, where each set has 2 points. The results are as below.

```
Scenario (a) - Constant line h(x) = b:
Average hypothesis: 0.33222032788657796
Bias: 0.08963788654539513
Variance: 0.043749727725588584
Risk: 0.13338761427098372
```

Analytically: Average hypothesis $= \frac{1}{3} \approx 0.3333$; Bias $= \frac{4}{45} \approx 0.0888$; Variance $= \frac{2}{45} \approx 0.0444$;

$$Risk = \frac{4}{45} + \frac{2}{45} = \frac{6}{45} \approx 0.1333$$

The analytically and numerically solution are pretty closed.

- (e) Now consider a line of the form $h(x) = ax + b$ which we fit by selecting the line that passes through our two observations. Modify the code from part (d) to estimate the new $\bar{h}(x)$, bias, variance, and risk. Explain how the results change and why.

The code is in HW5_1_e .

```
Scenario (b) - linear line h(x) = ax+b:
Average hypothesis a: -0.008069736345342441
Average hypothesis b: 0.0052214178466595375
Bias: 0.19466450093153284
Variance: 0.19786874186841863
Risk: 0.3925332427999515
```

Analytically: Average hypothesis $= \frac{1}{3} \approx 0.3333$; Bias $= \frac{4}{45} \approx 0.0888$; Variance $= \frac{2}{45} \approx 0.0444$;

$$\text{Risk} = \frac{4}{45} + \frac{2}{45} = \frac{6}{45} \approx 0.1333$$

For the analytically and numerically solution, the bias and the variances got much larger. This shows that linear estimator is not good for fitting $y = x^2$. The reason is if we use the average coefficient of $y = ax + b$ for 2 hypothesis points, the average slope a will turn to 0, because the $y = x^2$ is symmetric about the y -axis. For the same reason, the average constant b also turns to 0. Therefore, the final estimator would be like $y = 0$, which is obviously worse estimator than $y = b$ ($b = 0.33$) in previous question.

Problem 2: Let's consider the scenario described in Lecture 12, where x is drawn uniformly on the interval $[-1, 1]$ and $y = \sin(\pi x)$. We have $n = 2$ training samples: $(x_1, y_1), (x_2, y_2)$. Here we will look at an alternative approach to fitting a line to our data based on "Tikhonov regularization". In particular, we let

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \end{bmatrix} \quad \theta = \begin{bmatrix} b \\ a \end{bmatrix}$$

Then we consider Tikhonov regularized least squares estimators of the form

$$\hat{\theta} = (A^T A + \Gamma^T \Gamma)^{-1} A^T y \quad (1)$$

- (a) How would we set Γ to reduce this estimator to fitting a constant function (i.e., finding an $h(x) = b$)?

For this problem, it is sufficient to set Γ in a way that just makes $a \approx 0$. To make $a = 0$ exactly requires setting Γ in a way that makes the matrix $A^T A + \Gamma^T \Gamma$ singular – but note that this does not mean that the regularized least-squares optimization problem cannot be solved, you must just use a different formula than the one given in Eq.(1).

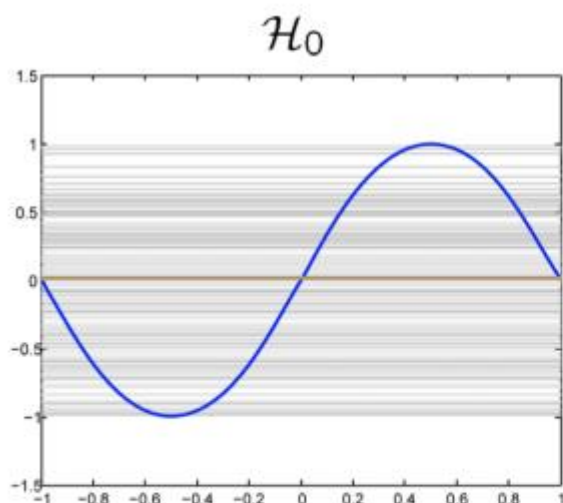
To let the estimator fitting the constant function, we set penalty factor γ very large, which prevents the estimator from having many features.

- (b) How would we set Γ to reduce this estimator to fitting a line $h(x) = ax + b$ that passes through the observed data points (i.e., $(x_1, y_1), (x_2, y_2)$)?

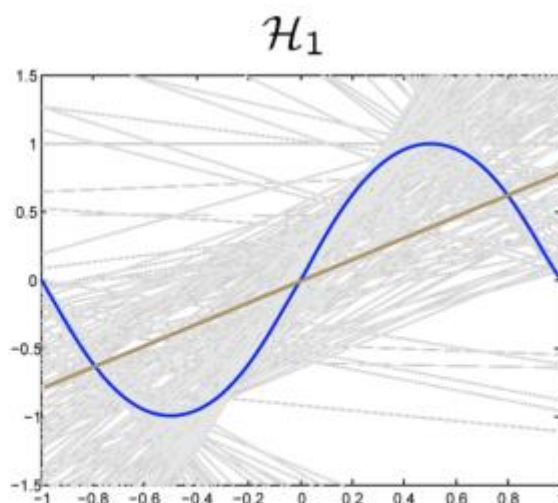
To let the estimator fitting a linear function, we set penalty factor γ less than the previous one, which will let the estimator has less punishment for features.

- (c) Estimate (numerically) the bias and variance for (at least approximations of) both of these estimators, and confirm that your estimates correspond to the numbers I provided in Lecture 13.

The code is in HW5_2_c .



bias = 0.50
variance = 0.25



bias \approx 0.21
variance \approx 1.69

```
bias_of_avg_theta_hat: 0.5002577355538642
avg_theta_hat: [0.02746831 0.00310861]
avg_predictions: [0.02763696 0.02721668]
overall_bias: 0.7520053927363686
overall_variance: 9.510887533817765e-06
```