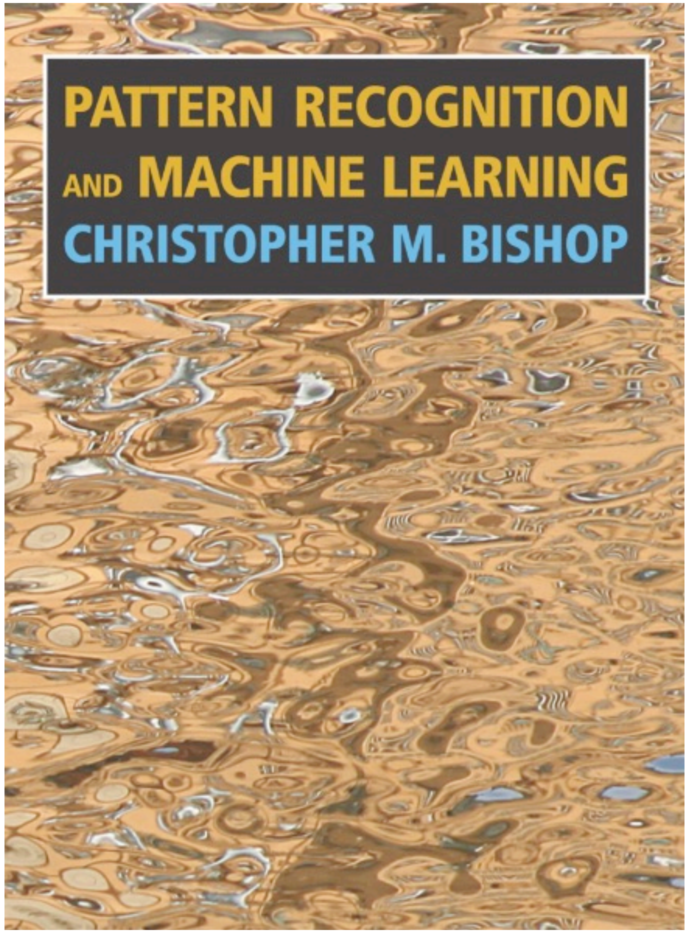
Bias-Variance Decomposition

Song Liu (song.liu@bristol.ac.uk)

Reference



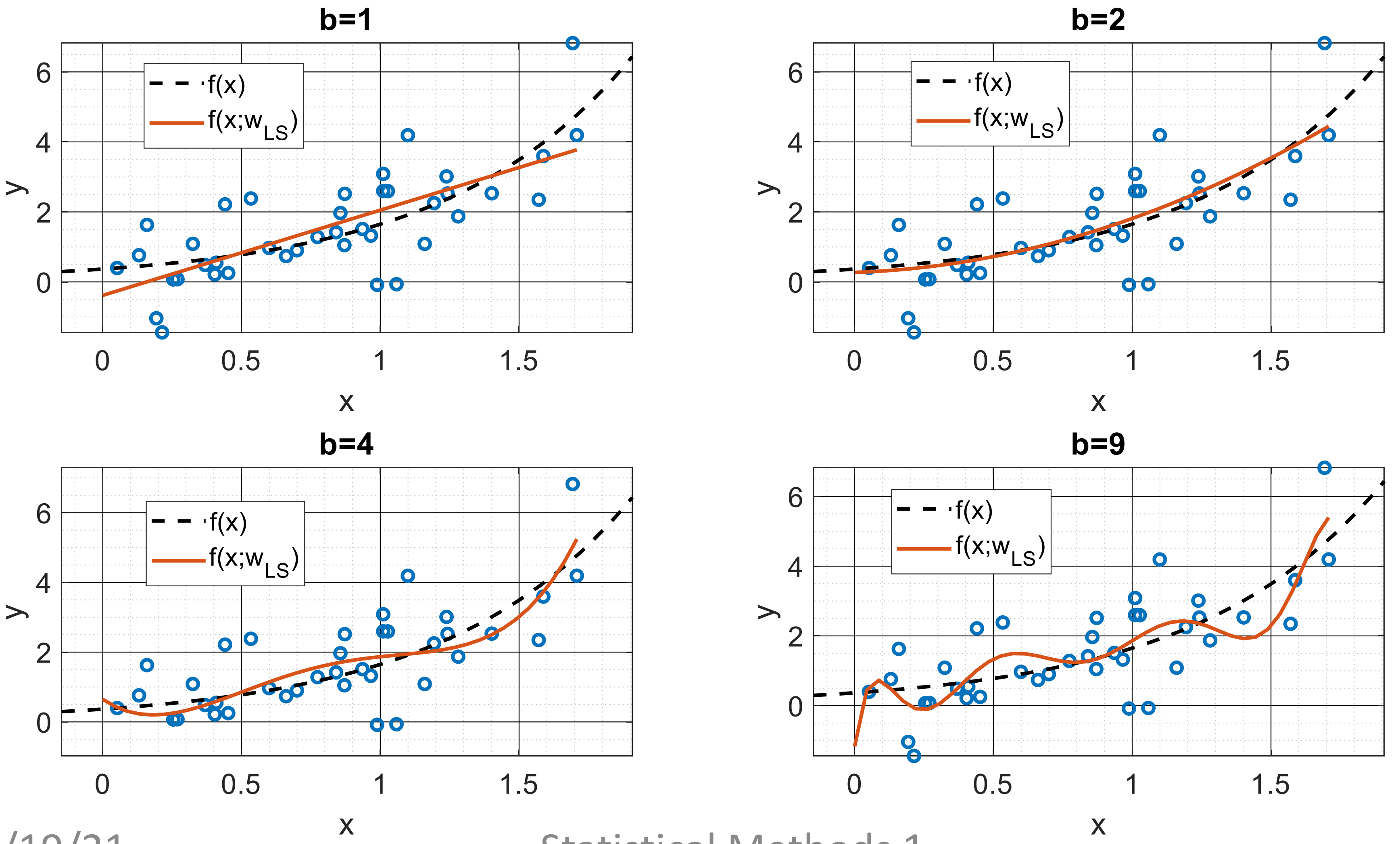
Today's class *roughly* follows Chapter 3.2.

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

Poly. Feature with various b

- $y = g(x) + \epsilon, g(x) = \exp(1.5x - 1), \epsilon \sim N(0, .64)$



What Really Happened?

- We mentioned that $f(\boldsymbol{x}; \boldsymbol{w}_{\text{LS}})$ is too flexible to generalize well on unobserved dataset, but why?
- What is the mathematical explanation of OF?
- Why testing error is a good measurement of the generalization of a prediction $f(\boldsymbol{x}; \boldsymbol{w}_{\text{LS}})$?

- We are introducing a frequentist analysis of explaining this phenomenon, called **Variance and Bias decomposition**.

From Testing Error to Expected Loss

- $E(D, \boldsymbol{w}_{\text{LS}})$ is the testing **error** of $\boldsymbol{w}_{\text{LS}}$ on a testing set D.
- We do not care $E(D, \boldsymbol{w}_{\text{LS}})$ on a specific testing dataset, let us take expectation with respect to D:

$$\mathbb{E}_D[E(D, w_{\text{LS}})] = \mathbb{E}_D\left[\sum_{i \in D}[y_i - f(\boldsymbol{x}_i; \boldsymbol{w}_{\text{LS}})]^2\right]$$

$$= \sum_{i=1..n} \underbrace{\mathbb{E}_D\left[[y - f(\boldsymbol{x}_i; \boldsymbol{w}_{\text{LS}})]^2 | \boldsymbol{x}_i\right]}_{\textbf{Expected Loss!}}$$

To investigate the expected loss further, we need to make some assumptions on the randomness of D.

Additive Noise Assumption

- First, assume an outcome y_i is generated by
- $y_i = g(\boldsymbol{x}_i) + \epsilon_i$.
  - $g(\boldsymbol{x}): R^d \to R$ is some deterministic function.
  - $\forall_i, \epsilon_i$ is independent of $\boldsymbol{x}_i$ and $\mathbb{E}[\epsilon_i] = 0$
  - We call ϵ_i **additive noise**.

- For example, if we assume ϵ_i comes from normal dist. with mean 0 and variance σ^2, y_i follows a normal distribution with mean $g(\boldsymbol{x}_i)$ and variance σ^2.

Decomposition of Expected Loss

- $\mathbb{E}_D\left[[y - f_{\mathrm{LS}}(\boldsymbol{x}_i)]^2 | \boldsymbol{x}_i\right] = \mathbb{E}_\epsilon\left[[y - f_{\mathrm{LS}}(\boldsymbol{x}_i)]^2 | \boldsymbol{x}_i\right]$

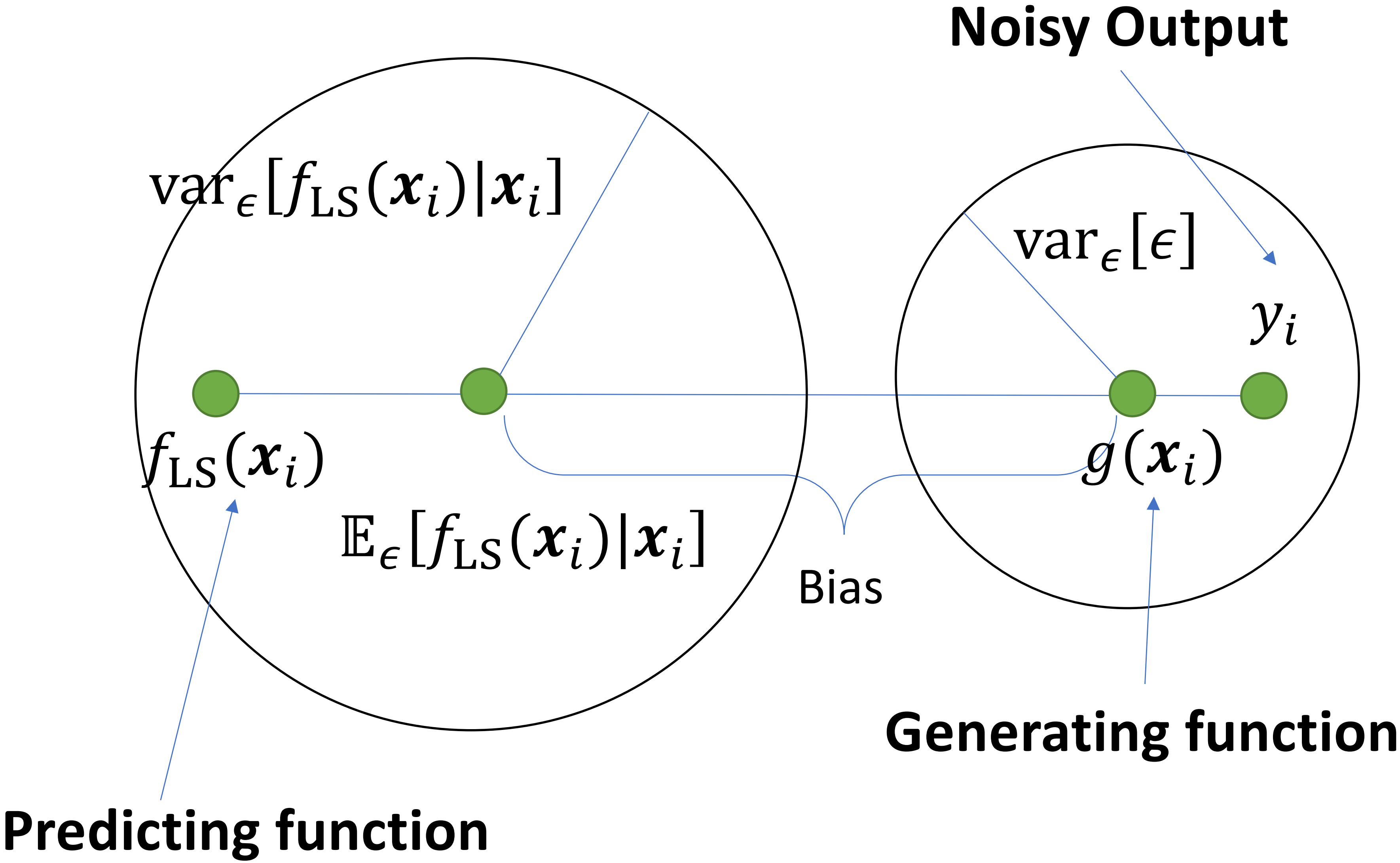
$$= \underbrace{\mathrm{var}_\epsilon[\epsilon]}_{\text{Irreducible error}} + \underbrace{\left[g(\boldsymbol{x}_i) - \mathbb{E}_\epsilon[f_{\mathrm{LS}}(\boldsymbol{x}_i) | \boldsymbol{x}_i]\right]^2}_{\text{bias}} + \underbrace{\mathrm{var}_\epsilon[f_{\mathrm{LS}}(\boldsymbol{x}_i) | \boldsymbol{x}_i}_{\text{variance}}$$

- "Variance and Bias decomposition"
- Prove it, hint, by our data generating assumption:
- $\mathbb{E}_\epsilon\left[[y - f_{\mathrm{LS}}(\boldsymbol{x}_i)]^2 | \boldsymbol{x}_i\right] = \mathbb{E}_\epsilon\left[[g(\boldsymbol{x}_i) + \epsilon - f_{\mathrm{LS}}(\boldsymbol{x}_i)]^2 | \boldsymbol{x}_i\right]$

“Variance and Bias decomposition”

- $\mathrm{var}[\epsilon] + \left[g(\boldsymbol{x}_i) - \mathbb{E}[f_{\mathrm{LS}}(\boldsymbol{x}_i)|\boldsymbol{x}_i]\right]^2 + \mathrm{var}[f_{\mathrm{LS}}(\boldsymbol{x}_i)|\boldsymbol{x}_i]$
    - 1st term measures the randomness of our data generating process, which is beyond our control.
    - 2nd term shows the accuracy of our expected prediction.
    - 3rd term shows how easily our fitted prediction function is affected by the randomness of the dataset.

A Visualization of V-B Decomposition

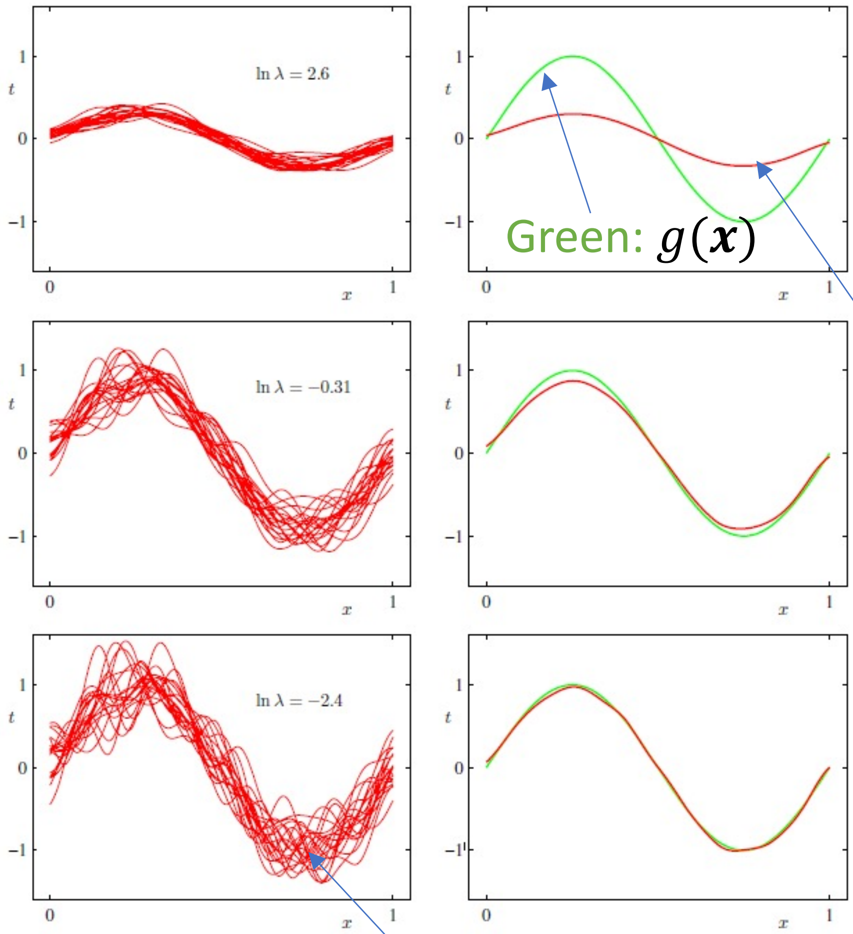


Variance and Bias Tradeoff

- $\mathrm{var}[\epsilon] + \left[g(\boldsymbol{x}_i) - \mathbb{E}[f_{\mathrm{LS}}(\boldsymbol{x}_i)|\boldsymbol{x}_i]\right]^2 + \mathrm{var}[f_{\mathrm{LS}}(\boldsymbol{x}_i)|\boldsymbol{x}_i]$

  - As we increase b, f_{LS} becomes more **complex** and can adapt to more complex underlying function, thus 2nd term keeps reducing.
  - As we increase b, f_{LS} becomes more **sensitive** to the noise in our dataset, thus 3rd term keeps increasing.
  - A **balance** between 2nd and 3rd term gives the minimum expected error.

Variance and Bias Tradeoff



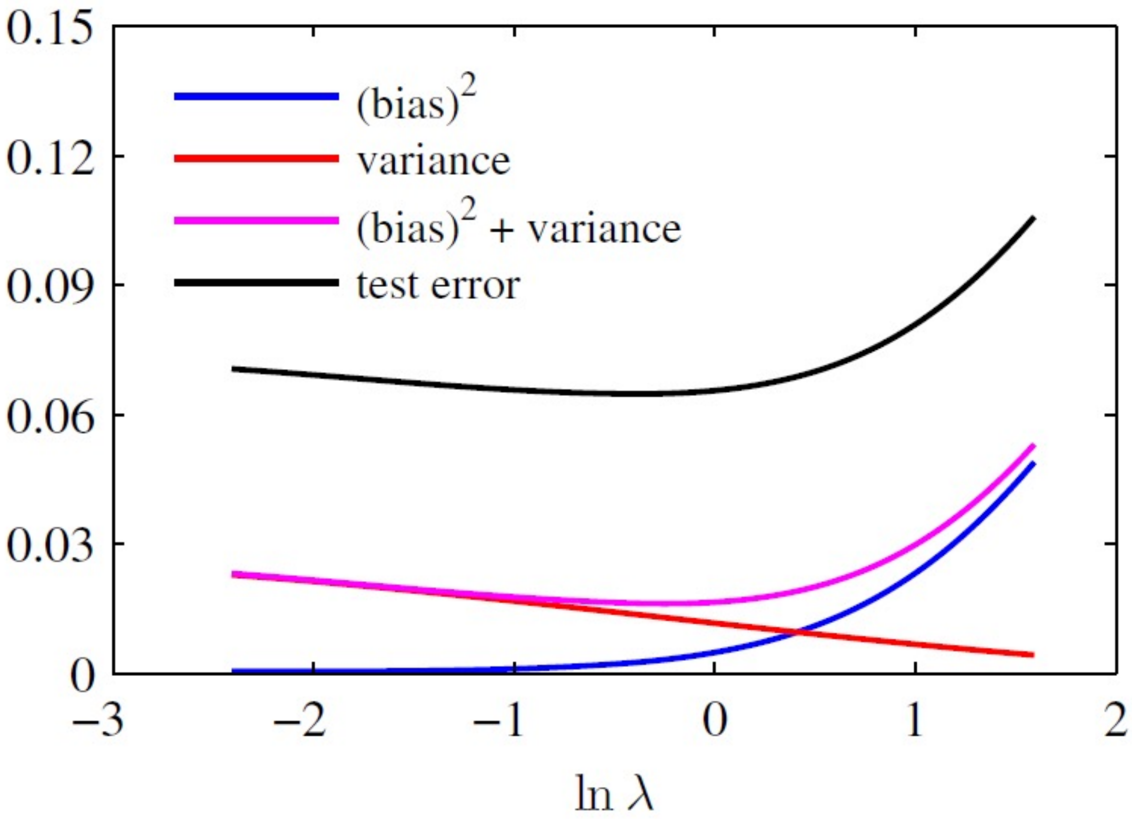
- As flexibility increases (λ decreases), the bias decreases, and the variance increases.

Red: **Expected** f_{LS}

PRML Figure 3.5

Red: f_{LS} over different datasets, see the variances

Variance and Bias Tradeoff



PRML Figure 3.6

- As the flexibility decreases (λ increase), bias increases and the variance decreases.

In-Sample Error

- $\mathbb{E}_\epsilon[(y - f_{\text{LS}}(\boldsymbol{x}_i))^2 | \boldsymbol{x}_i]$ is conditional on $\boldsymbol{x}_i$.
- To calculate the collective error, we need to average over all $\boldsymbol{x}_i$.
  - $\frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_\epsilon[(y - f_{\text{LS}}(\boldsymbol{x}_i))^2 | \boldsymbol{x}_i]$
  - is called **in sample error**

- Can we use in sample error to measure the performance of our f_{LS}?

Out-Sample Error

- In sample error is not useful in practice.
  - We cannot calculate $\mathbb{E}_{\epsilon}[(y - f_{\mathrm{LS}}(\boldsymbol{x}_i))^2 | \boldsymbol{x}_i]$
  - We do not know $g(\boldsymbol{x})$ and the distribution of ϵ.
- Instead, we use **out-sample error**:
  - Error over the entire distribution of $\boldsymbol{x}$:
  - $\boxed{\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{\epsilon}[(y - f_{\mathrm{LS}}(\boldsymbol{x}))^2 | \boldsymbol{x}]}$
  - $$\begin{aligned}\mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{\epsilon}[(y - f_{\mathrm{LS}}(\boldsymbol{x}))^2 | \boldsymbol{x}] &= \mathbb{E}_{\boldsymbol{x}}\mathbb{E}_{y}[(y - f_{\mathrm{LS}}(\boldsymbol{x}))^2 | \boldsymbol{x}] \\ &= \mathbb{E}_{p(y,\boldsymbol{x})}[(y - f_{\mathrm{LS}}(\boldsymbol{x}))^2]\end{aligned}$$

- Can we approximate out-sample error?

Approx. Out-Sample Error

- Train least-squares on dataset D_0, getting f_0 ,
- Obtain a fresh batch datapoints $D_1 := \{(y_i', \boldsymbol{x}_i') \}_{i=1}^{n'}$,
- D_1 and D_0 are independently and identically distributed:
- $\frac{1}{n'}\sum_{(y',\boldsymbol{x}')\in D_1}\left(y' - f_0(\boldsymbol{x}')\right)^2 \approx \mathbb{E}_{p(y,\boldsymbol{x})}[(y - f_0(\boldsymbol{x}))^2]$
  - due to law of large numbers.
- $\mathbb{E}_{p(y,\boldsymbol{x})}[(y - f_0(\boldsymbol{x}))^2] \approx \mathbb{E}_{p(y,\boldsymbol{x})}[(y - f_{\mathrm{LS}}(\boldsymbol{x}))^2]$

- $\frac{1}{n'}\sum_{(y',\boldsymbol{x}')\in D_1}(y' - f_0(\boldsymbol{x}'))^2$ is $E(D_1, f_0)$!
- This justifies the usage of $E(D_1, f_0)$ for evaluating the overfitting of our prediction f_0.

Conclusion

- The phenomenon of OF can be explained by decomposition of expected error.
- Two types of expected errors can be used for measuring the performance of f_{LS}:
  - In-sample error, cannot be computed, unless we know g and dist. of ϵ.
  - Out-sample error, can be roughly approximated by $E(D_1, f_0)$, which is the testing error.

Homework

- Prove variance and bias decomposition.
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