Module 8.2 : Train error vs Test error

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- See proof here

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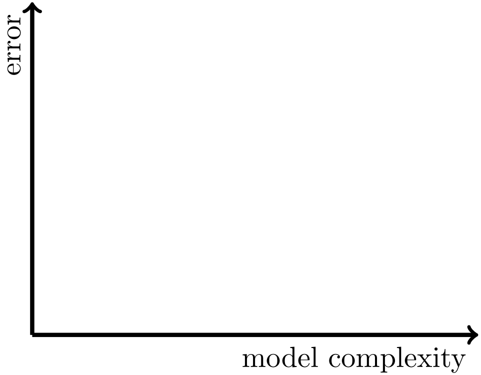

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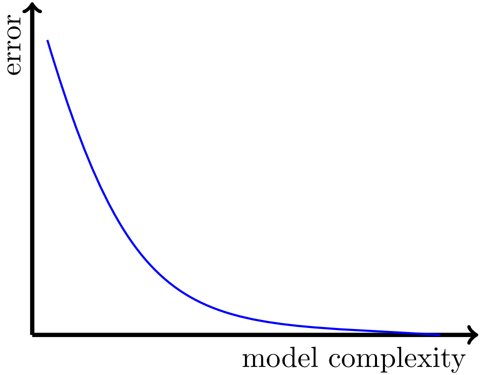

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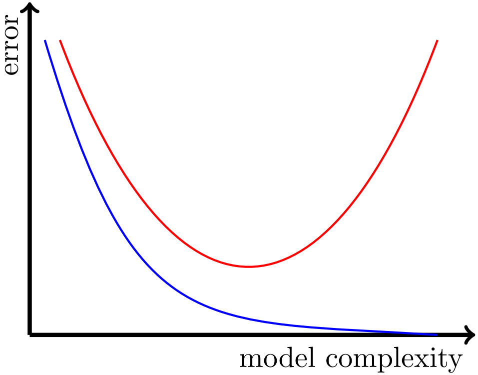

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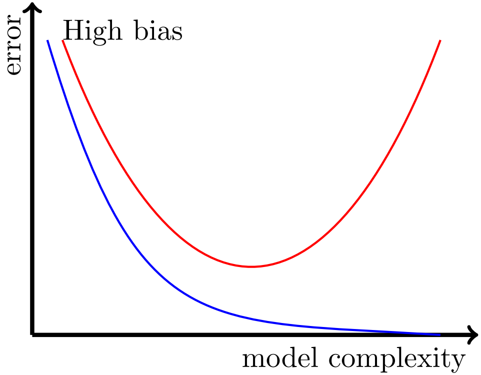

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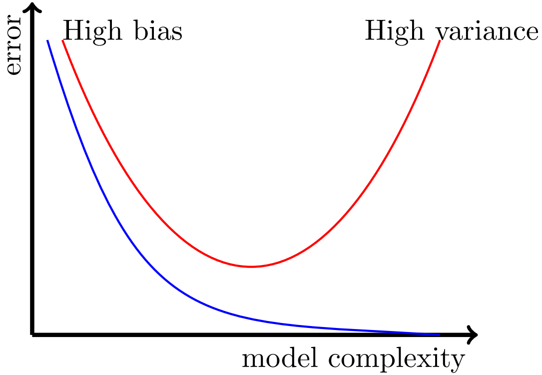

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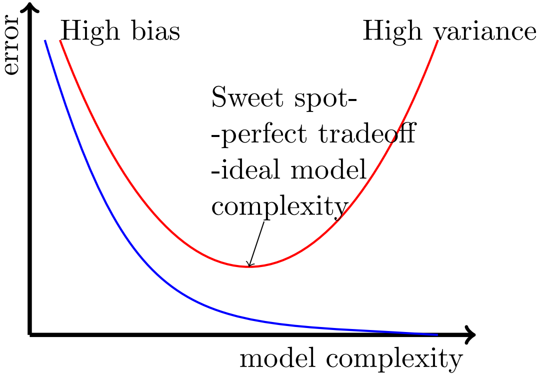

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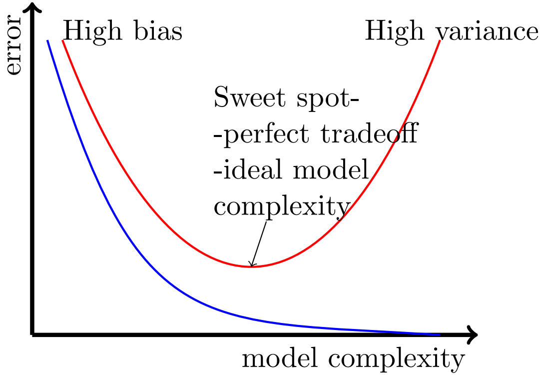

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- We will concretize this intuition mathematically now and eventually show how to account for the optimism in the training error

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- We will see how to estimate this empirically using the observation y_i & prediction $\hat{y}_i$

$$E[(\hat{y}_i - y_i)^2]$$

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E[(\hat{y}_i - y_i)^2] &= E[(\hat{f}(x_i) - f(x_i) - \varepsilon_i)^2] \quad \color{red}{(y_i = f(x_i) + \varepsilon_i)} \\
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$$\therefore E[(\hat{f}(x_i) - f(x_i))^2] \;=\; E[(\hat{y}_i - y_i)^2] \;-\; E[\varepsilon_i^2] \;+\; 2E[\,\varepsilon_i(\hat{f}(x_i) - f(x_i))\,]$$

We will take a small detour to understand how to empirically estimate an Expectation and then return to our derivation

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$$E[(\hat{y}_i - y_i)^2] = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2$$

... returning back to our derivation

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- We can empirically evaluate R.H.S using training observations or test observations

Case 1: Using test observations

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$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\,error}$$

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$\because$ covariance(X, Y)

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$$\begin{aligned} \because \text{covariance}(X,Y) &= E[(X-\mu_X)(Y-\mu_Y)] \\ &= E[(X)(Y-\mu_Y)](\text{if } \mu_X = E[X] = 0) \\ &= E[XY] - E[X\mu_Y] = E[XY] - \mu_Y E[X] = E[XY] \end{aligned}$$

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error}$$

$$= \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=\ covariance\,(\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

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- None of the test observations participated in the estimation of $\hat{f}(x)$[the parameters of $\hat{f}$(x) were estimated only using training data]

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$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))] = E[\varepsilon_i] \cdot E[\hat{f}(x_i) - f(x_i))]$$

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error}$$

$$= \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{m}\sum_{i=n+1}^{n+m}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=\ covariance\ (\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

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$$\therefore \text{true error} = \text{empirical test error} + \text{small constant}$$

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$$\therefore \text{true error} = \text{empirical test error} + \text{small constant}$$

- Hence, we should always use a validation set(independent of the training set) to estimate the error

Case 2: Using training observations

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error}$$

$$= \underbrace{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{n}\sum_{i=1}^{n}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{= covariance\,(\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

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Now, $\varepsilon \not\perp \hat{f}(\text{x})$ because ε was used for estimating the parameters of $\hat{f}(x)$

$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))]$$

Case 2: Using training observations

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Now, $\varepsilon \not\perp \hat{f}(\mathrm{x})$ because ε was used for estimating the parameters of $\hat{f}(x)$

$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))] \neq E[\varepsilon_i] \cdot E[\hat{f}(x_i) - f(x_i))]$$

Case 2: Using training observations

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error} = \underbrace{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{n}\sum_{i=1}^{n}\varepsilon_i^2}_{small\ constant} + 2\underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{= covariance\,(\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

Now, $\varepsilon \not\perp \hat{f}(\mathrm{x})$ because ε was used for estimating the parameters of $\hat{f}(x)$

$$\therefore E[\varepsilon_i \cdot (\hat{f}(x_i) - f(x_i))] \neq E[\varepsilon_i] \cdot E[\hat{f}(x_i) - f(x_i))] \neq 0$$

Hence, the empirical train error is smaller than the true error and does not give a true picture of the error

Case 2: Using training observations

$$\underbrace{E[(\hat{f}(x_i) - f(x_i))^2]}_{true\ error} = \underbrace{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}_{empirical\ estimation\ of\ error} - \underbrace{\frac{1}{n}\sum_{i=1}^{n}\varepsilon_i^2}_{small\ constant} + 2\ \underbrace{E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]}_{=covariance\,(\varepsilon_i, \hat{f}(x_i) - f(x_i))}$$

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Hence, the empirical train error is smaller than the true error and does not give a true picture of the error

But how is this related to model complexity? Let us see