Module 8.2 : Train error vs Test error

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(average square error in predicting y for many such unseen points)

- We can show that

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- See proof here

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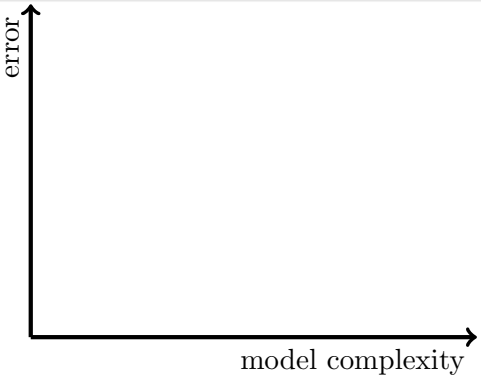

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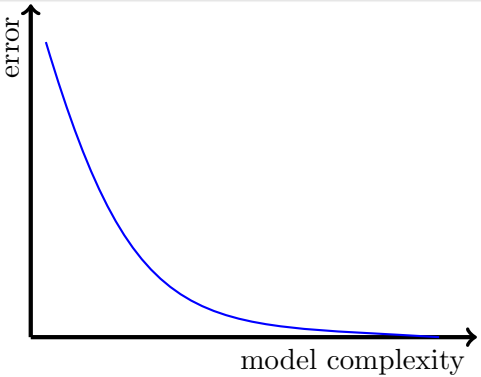

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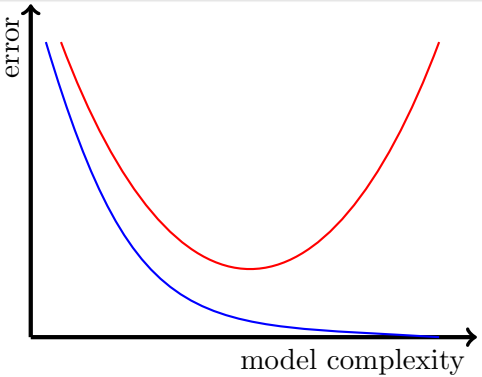

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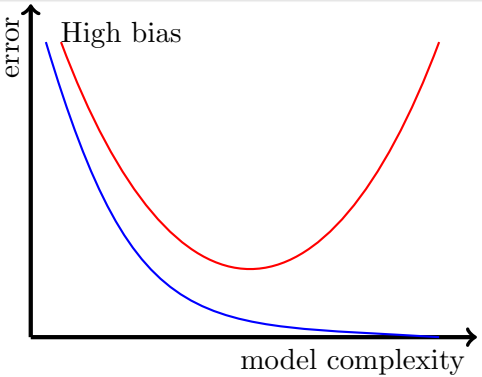

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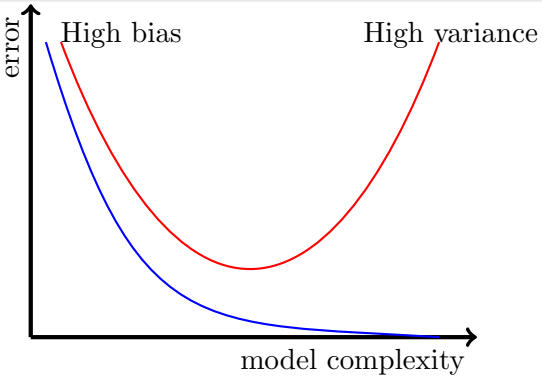

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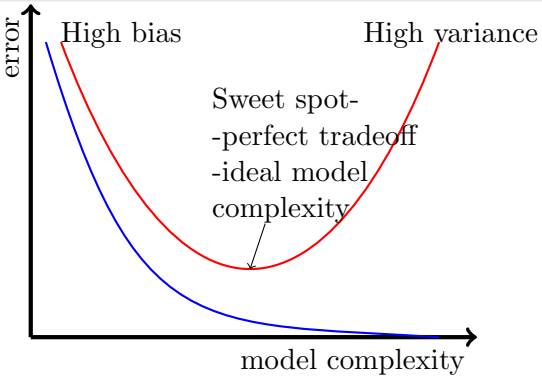

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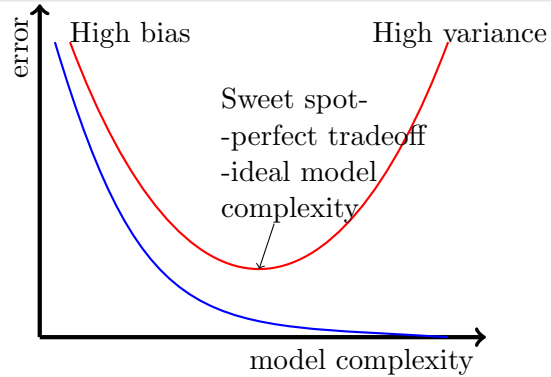

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- Let there be n training points and m test (validation) points

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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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$$\therefore E[(\hat{f}(x_i) - f(x_i))^2] = E[(\hat{y}_i - y_i)^2] - E[\varepsilon_i^2] + 2E[\ \varepsilon_i(\hat{f}(x_i) - f(x_i))\ ]$$

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

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

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

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

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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

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