- We can show that

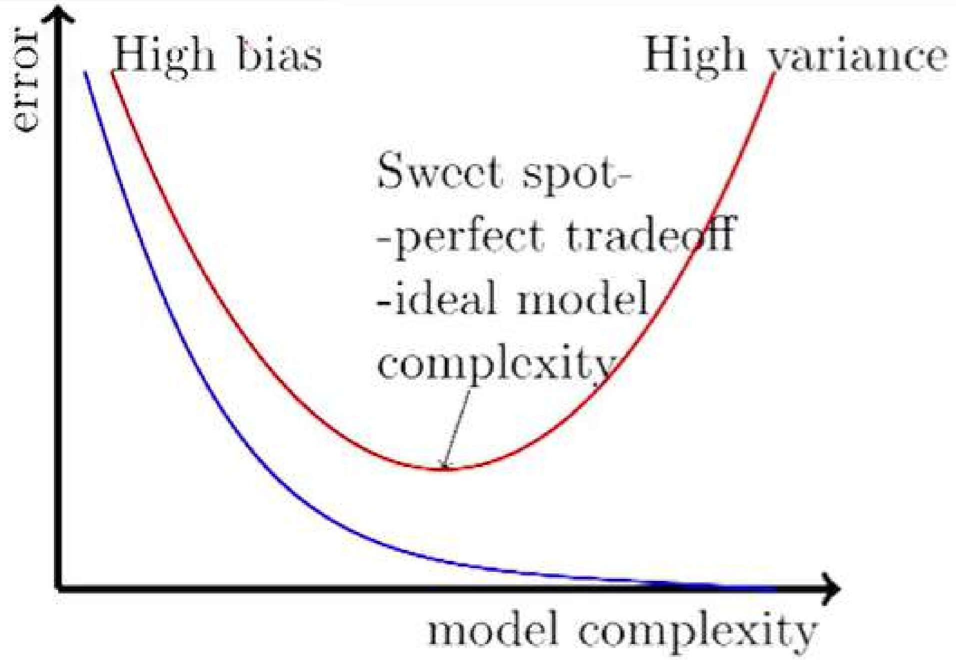
$$E[(y - \hat{f}(x))^2] = Bias^2 + Variance + \sigma^2 \text{ (irreducible error)}$$

- See proof here

- Consider a new point (x, y) which was not seen during training
- If we use the model $\hat{f}(x)$ to predict the value of y then the mean square error is given by

$$E[(y - \hat{f}(x))^2]$$

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



$$E[(y - \hat{f}(x))^2] = Bias^2 + Variance + \sigma^2 \text{ (irreducible error)}$$

- The parameters of $\hat{f}(x)$ (all w_i's) are trained using a training set $\{(x_i, y_i)\}_{i=1}^n$
- However, at test time we are interested in evaluating the model on a validation (unseen) set which was not used for training
- This gives rise to the following two entities of interest:
  $train_{err}$ (say, mean square error)
  $test_{err}$ (say, mean square error)
- Typically these errors exhibit t
  in the adjacent figure

Intuitions developed so far

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

$$train_{err} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

$$test_{err} = \frac{1}{m}\sum_{i=n+1}^{n+m}(y_i - \hat{f}(x_i))$$

- As the model complexity increases $train_{err}$ becomes overly optimistic and gives us a wrong picture of how close $\hat{f}$ is to f
- The validation error gives the real picture of how close $\hat{f}$ is to f
- We will concretize this intuition mathematically now and eventually show how to account for the optimism in the training error

- Let D=$\{x_i, y_i\}_{i=1}^{m+n}$, then for any point (x, y) we have,

$$y_i = f(x_i) + \varepsilon_i$$

- which means that y_i is related to x_i by some true function f but there is also some noise ε in the relation

- For simplicity, we assume

$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

and of course we do not know f

- Further we use $\hat{f}$ to approximate f and estimate the parameters using T $\subset$ D such that

$$y_i = \hat{f}(x_i)$$

- We are interested in knowing

$$E[(\hat{f}(x_i) - f(x_i))^2]$$

but we cannot estimate this directly because we do not know f

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

9:02 / 11:23

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

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

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

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

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

- Suppose we have observed the goals scored(z) in k matches as $z_1 = 2,\ z_2 = 1,\ z_3 = 0,\ \ldots\ z_k = 2$
- Now we can empirically estimate $E[z]$ i.e. the expected number of goals scored as

$$E[z] = \frac{1}{k}\sum_{i=1}^{k} z_i$$

- Analogy with our derivation: We have a certain number of observations y_i & predictions $\hat{y}_i$ using which we can estimate

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

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

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

Case 1: Using test observations

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

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

10:14 / 18:00

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

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

- 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]

$$\therefore \varepsilon \perp (\hat{f}(x_i) - f(x_i))$$

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

$\therefore$ true error = empirical test error + small constant

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

15:31 / 18:00

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, $\varepsilon \not\perp \hat{f}$(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