

## Bias - Variance Tradeoff

True data generated from noisy model  $\vec{y} = f(x) + \vec{\epsilon}$  with  $\vec{\epsilon} \approx \mathcal{N}(0, \sigma^2)$

Approximate  $f$  by the model:  $\tilde{y} = X\hat{\beta}$

with  $\hat{\beta}$  optimal parameters minimizing  $C(X, \beta) = \mathbb{E}[(y - \tilde{y})^2] = \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2$

Therefore:

$$C = \mathbb{E}[(y - \tilde{y})^2]$$

$$= \mathbb{E}[(f + \epsilon - \tilde{y})^2]$$

$$= \mathbb{E}[(f - \tilde{y})^2 + 2\epsilon \cdot (f - \tilde{y}) + \epsilon^2]$$

$$= \mathbb{E}[(f - \tilde{y})^2] + \mathbb{E}[\epsilon^2]$$

$$= \mathbb{E}[(f - \tilde{y})^2] + \sigma^2$$

$$\mathbb{E}[\epsilon] = 0$$

$$\text{var}[\epsilon] = \mathbb{E}[\epsilon^2] - \mathbb{E}[\epsilon]^2 = \sigma^2$$

$$\sigma^2 = \mathbb{E}[\epsilon^2]$$

Adding and subtracting

$$= \mathbb{E}[(f + \mathbb{E}[\tilde{y}] - \tilde{y} - \mathbb{E}[\tilde{y}])^2] + \sigma^2$$

$$= \mathbb{E}[(f - \mathbb{E}[\tilde{y}] - (\tilde{y} - \mathbb{E}[\tilde{y}]))^2] + \sigma^2$$

Expanding

$$= \mathbb{E}[(f - \mathbb{E}[\tilde{y}])^2 + (\tilde{y} - \mathbb{E}[\tilde{y}])^2 - 2(f - \mathbb{E}[\tilde{y}]) \cdot (\tilde{y} - \mathbb{E}[\tilde{y}])] + \sigma^2$$

$$= \mathbb{E}[(f - \mathbb{E}[\tilde{y}])^2] + \mathbb{E}[(\tilde{y} - \mathbb{E}[\tilde{y}])^2] - 2 \underbrace{\mathbb{E}[(f - \mathbb{E}[\tilde{y}]) \cdot (\tilde{y} - \mathbb{E}[\tilde{y}])]}_{\text{NON-STOCHASTIC}} + \sigma^2$$

$$C = \mathbb{E}[(f - \mathbb{E}[\tilde{y}])^2] + \mathbb{E}[(\tilde{y} - \mathbb{E}[\tilde{y}])^2] - 2(f - \mathbb{E}[\tilde{y}]) \cdot \underbrace{\mathbb{E}[\tilde{y} - \mathbb{E}[\tilde{y}]]}_{=0} + \sigma^2$$

$$\text{Note } \mathbb{E}[y] = \mathbb{E}[f + \epsilon] = f$$

$$\text{Then } C(X, \beta) = \mathbb{E}[(\mathbb{E}[y] - \mathbb{E}[\tilde{y}])^2] + \mathbb{E}[(\tilde{y} - \mathbb{E}[\tilde{y}])^2] + \sigma^2$$

$$\equiv \text{Bias}[\tilde{y}] + \text{var}[\tilde{y}] + \sigma^2$$

$\sigma^2$ : Unavoidable error arising from the error in the experimental data  $\vec{y}$  (noisy model)

$\text{Bias}[\tilde{y}]$ : Indicates how far the mean values of the experimental data  $\vec{y}$  and the model  $\tilde{y}$  are, on average.

$\text{var}[\tilde{y}]$ : Measures the average distance that the values of the  $\tilde{y}(x)$  model deviate from their mean value. Indicates how spread out the model's data is.