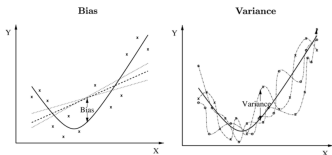


# Introduction to Machine Learning

## Bias-Variance Decomposition

### Learning goals



- Understand how to decompose the generalization error of an inducer into
  - Bias of the inducer
  - Variance of the inducer
  - Noise in the data

# BIAS-VARIANCE DECOMPOSITION

Let us take a closer look at the generalization error of a learning algorithm  $\mathcal{I}_{L,O}$ . This is the expected error an induced model, on trainings sets of size  $n$ , when this is applied to a fresh, random test observation.

$$GE_n(\mathcal{I}_{L,O}) = \mathbb{E}_{\mathcal{D}_n \sim \mathbb{P}_{xy}, (\mathbf{x}, y) \sim \mathbb{P}_{xy}} \left( L \left( y, \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right) = \mathbb{E}_{\mathcal{D}_n, xy} \left( L \left( y, \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)$$

We therefore need to take the expectation over all training sets of size  $n$ , as well as the independent test observation.

We assume that the data is generated by

$$y = f_{\text{true}}(\mathbf{x}) + \epsilon,$$

with normally distributed error  $\epsilon \sim \mathcal{N}(0, \sigma^2)$  independent of  $\mathbf{x}$ .

# BIAS-VARIANCE DECOMPOSITION

By plugging in the  $L2$  loss  $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$  we get

$$\begin{aligned} GE_n(\mathcal{I}_{L,O}) &= \mathbb{E}_{\mathcal{D}_n, xy} \left( L(y, \hat{f}_{\mathcal{D}_n}(\mathbf{x})) \right) = \mathbb{E}_{\mathcal{D}_n, xy} \left( (y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \right) \\ &= \mathbb{E}_{xy} \underbrace{\left[ \mathbb{E}_{\mathcal{D}_n} \left( (y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \mid \mathbf{x}, y \right) \right]}_{(*)} \end{aligned}$$

Let us consider the error  $(*)$  conditioned on one fixed test observation  $(\mathbf{x}, y)$  first. (We omit the  $\mid \mathbf{x}, y$  for better readability for now.)

$$\begin{aligned} (*) &= \mathbb{E}_{\mathcal{D}_n} \left( (y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}))^2 \right) \\ &= \underbrace{\mathbb{E}_{\mathcal{D}_n} (y^2)}_{=y^2} + \underbrace{\mathbb{E}_{\mathcal{D}_n} (\hat{f}_{\mathcal{D}_n}(\mathbf{x})^2)}_{(1)} - 2 \underbrace{\mathbb{E}_{\mathcal{D}_n} (y \hat{f}_{\mathcal{D}_n}(\mathbf{x}))}_{(2)} \end{aligned}$$

by using the linearity of the expectation.

# BIAS-VARIANCE DECOMPOSITION

$$\mathbb{E}_{\mathcal{D}_n} \left( \left( y - \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)^2 \right) = y^2 + \underbrace{\mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x})^2 \right)}_{(1)} - 2 \underbrace{\mathbb{E}_{\mathcal{D}_n} \left( y \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)}_{(2)} =$$

By using that  $\mathbb{E}(z^2) = \text{Var}(z) + \mathbb{E}^2(z)$ , we see that

$$= y^2 + \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \mathbb{E}_{\mathcal{D}_n}^2 \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) - 2y \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)$$

Plug in the definition of  $y$

$$= f_{\text{true}}(\mathbf{x})^2 + 2\epsilon f_{\text{true}}(\mathbf{x}) + \epsilon^2 + \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \mathbb{E}_{\mathcal{D}_n}^2 \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) - 2(f_{\text{true}}(\mathbf{x}) + \epsilon) \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)$$

Reorder terms and use the binomial formula

$$= \epsilon^2 + \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)^2 + 2\epsilon \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)$$

# BIAS-VARIANCE DECOMPOSITION

$$(*) = \epsilon^2 + \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) + \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)^2 + 2\epsilon \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right) \right)$$

Let us come back to the generalization error by taking the expectation over all fresh test observations  $(\mathbf{x}, y) \sim \mathbb{P}_{xy}$ :

$$\begin{aligned} GE_n(\mathcal{I}_{L,O}) &= \underbrace{\sigma^2}_{\text{Variance of the data}} + \underbrace{\mathbb{E}_{xy} \left[ \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \mid \mathbf{x}, y \right) \right]}_{\text{Variance of inducer at } (\mathbf{x}, y)} \\ &+ \underbrace{\mathbb{E}_{xy} \left[ \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)^2 \mid \mathbf{x}, y \right) \right]}_{\text{Squared bias of inducer at } (\mathbf{x}, y)} + \underbrace{0}_{\text{As } \epsilon \text{ is zero-mean and independent}} \end{aligned}$$

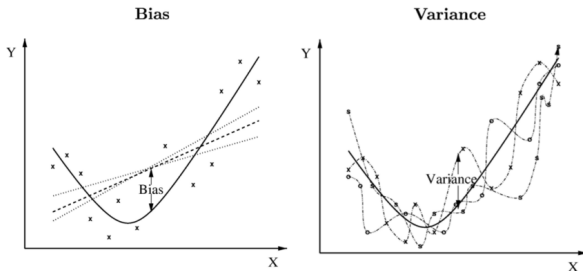
# BIAS-VARIANCE DECOMPOSITION

$$GE_n(\mathcal{I}_{L,O}) =$$

$$\underbrace{\sigma^2}_{\text{Variance of the data}} + \underbrace{\mathbb{E}_{xy} \left[ \text{Var}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \mid \mathbf{x}, y \right) \right]}_{\text{Variance of inducer at } (\mathbf{x}, y)} + \underbrace{\mathbb{E}_{xy} \left[ \left( f_{\text{true}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}_n} \left( \hat{f}_{\mathcal{D}_n}(\mathbf{x}) \right)^2 \mid \mathbf{x}, y \right) \right]}_{\text{Squared bias of inducer at } (\mathbf{x}, y)}$$

- ❶ The first term expresses the variance of the data. This is **noise** present in the data. Also called Bayes, intrinsic or unavoidable error. No matter what we do, we will never get below this error.
- ❷ The second term expresses how the predictions fluctuate on test-points on average, if we vary the training data. Expresses also the learner's tendency to learn random things irrespective of the real signal (overfitting).
- ❸ The third term says how much we are "off" on average at test locations (underfitting). Models with high capacity have low **bias** and models with low capacity have high **bias**.

# BIAS-VARIANCE DECOMPOSITION



**Figure:** *Left:* A model with high bias is unable to fit the curved relationship present in the data. *Right:* A model with no bias and high variance can, in principle, learn the true pattern in the data. However, in practice, the learner outputs wildly different hypotheses for different training sets.