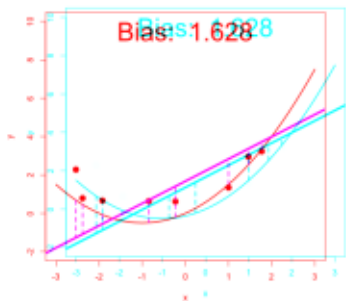


Introduction to Machine Learning

Advanced Risk Minimization: Bias-Variance Decomposition



Learning goals

- Understand how to decompose the generalization error of a learner into
 - bias of the learner
 - variance of the learner
 - inherent noise in the data
 - variance of the learner
 - inherent noise in the data

BIAS-VARIANCE DECOMPOSITION

Let us take a closer look at the generalization error of a learning algorithm \mathcal{I}_L . This is the expected error of an induced model $\hat{f}_{\mathcal{D}_n}$, on training sets of size n , when applied to a fresh, random test observation.

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

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

For the squared loss, there is a nice additive decomposition of $GE_n(\mathcal{I}_L)$ into three components. \mathbf{x} is generated by

Hence we assume that the data is generated by

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

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with zero-mean homoskedastic error $\epsilon \sim (0, \sigma^2)$ independent of \mathbf{x} .

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* Similar decomp's also exist for other losses expressible as Bregman divergences (e.g. cross-entropy). One exception is the 0/1 loss (Brown and Ali 2024)



BIAS-VARIANCE DECOMPOSITION / 2

$$GE_n(\mathcal{I}_L) =$$

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



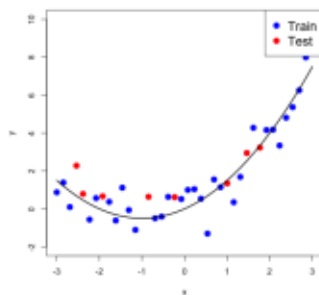
- 1 The first term expresses the variance of the data. This is pure **noise** in the data. Also called Bayes, intrinsic or irreducible error. No matter what we do, we will never get below this error.
- 2 The second term expresses, on average, how much $\hat{f}_{\mathcal{D}_n}(\mathbf{x})$ fluctuates around test points if we vary the training data. Expresses also the learner's tendency to learn random things irrespective of the real signal (overfitting).
- 3 The third term says how much we are "off" on average at test locations (underfitting). Models with high capacity typically have low **bias** and *vice versa*.

BIAS-VARIANCE DECOMPOSITION / 3

Illustration: Let us consider the following example. We will generate a dataset using the following model :

$$y = x + \frac{x^2}{2} + \epsilon, \quad \epsilon \sim N(0, 1)$$

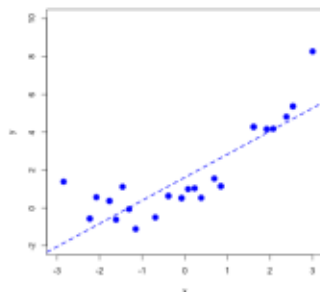
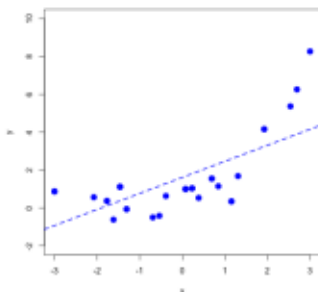
The data is then split into a training set and a test set.



BIAS-VARIANCE DECOMPOSITION / 4

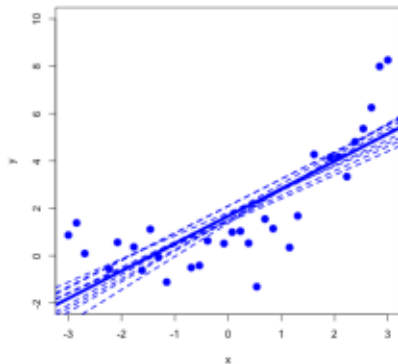
To obtain estimates for the bias and variance, we will train several models by sampling with replacement from the training data. This is commonly known as **bootstrapping**.

First, we train several (low capacity) linear models (polynomial of degree $d = 1$).



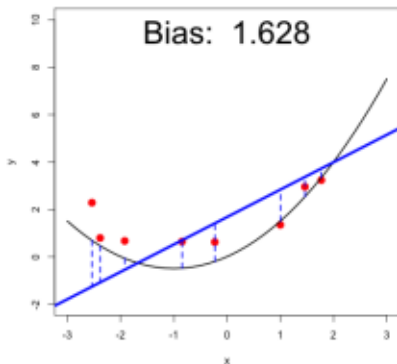
BIAS-VARIANCE DECOMPOSITION / 5

By creating several models, we obtain the average model over different samples of the training dataset.



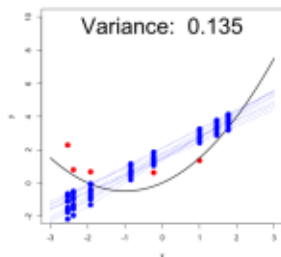
BIAS-VARIANCE DECOMPOSITION / 6

We can now estimate the (squared) bias, by computing the average squared difference between the average model and the true model, at the test point locations.



BIAS-VARIANCE DECOMPOSITION / 7

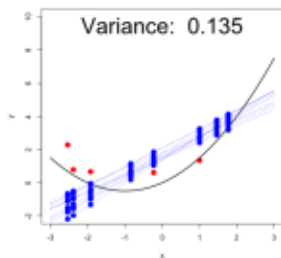
We compute the average variance of the predictions of the models we trained at the test point locations.



$$GE_n(\mathcal{I}_L) \approx 1 + 1.628 + 0.135 = 2.763$$

- The biggest component of the generalization error is the bias.
- Computing the MSE in the usual way for each model, via L2 loss, and then averaging over models gives rise to nearly the same value, as expected

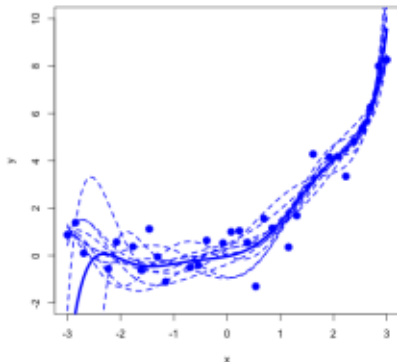
BIAS-VARIANCE DECOMPOSITION / 8



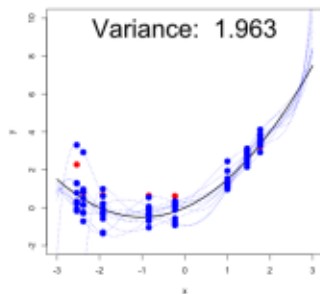
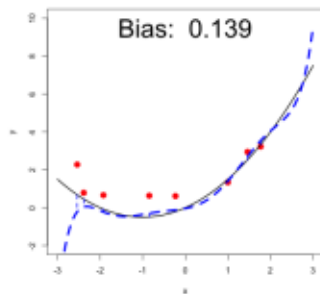
- We can now check whether this alternative computation of the GE is correct
- So, we simply compute the MSE in the standard fashion for each model
- So for each model we compute the L2 loss at each data point, then average
- Then we average these MSEs over all models
- Result = 2.72, would be closer if we average over more models and test points

BIAS-VARIANCE DECOMPOSITION / 9

We will repeat the same procedure, but use a high-degree polynomial ($d = 7$) with more capacity.



BIAS-VARIANCE DECOMPOSITION / 10

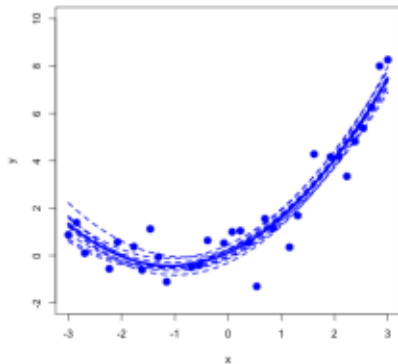


$$GE_n(\mathcal{I}_L) \approx 1 + 0.139 + 1.963 = 3.102$$

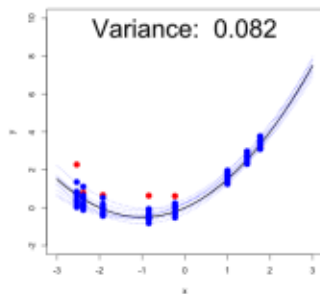
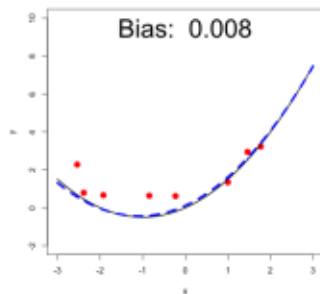
- The generalization error is higher than before
- Even though the bias is lower, the variance of the learner is higher.

BIAS-VARIANCE DECOMPOSITION / 11

What happens if we use a model with the same complexity as the true model (quadratic polynomial)?



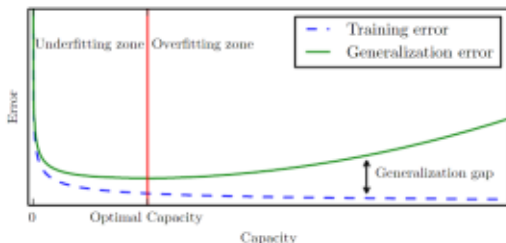
BIAS-VARIANCE DECOMPOSITION / 12



$$GE_n(\mathcal{I}_L) \approx 1 + 0.008 + 0.082 = 1.091$$

- The generalization error is the lowest at this complexity.
- The variance of the data acts as a lower bound.

CAPACITY AND OVERFITTING

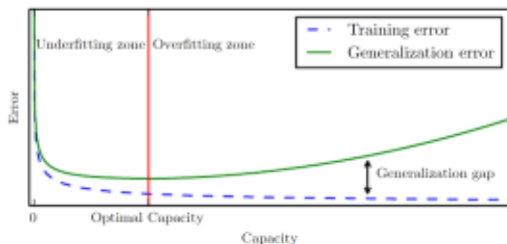


Credit: Ian Goodfellow



- The performance of a learner depends on its ability to
 - 1 **fit** the training data well
 - 2 **generalize** to new data
- Failure of the first point is called **underfitting**
- Failure of the second item is called **overfitting**

CAPACITY AND OVERFITTING / 2



Credit: Ian Goodfellow



- The tendency of a model to underfit/overfit is a function of its capacity, determined by the type of hypotheses it can learn.
- Usually, low bias means high capacity, which in turn means a higher chance of overfitting
- Low-bias models usually have also higher variance
- For such models, regularization (we discuss later) is essential
- Even for correctly specified models, the generalization error is lower-bounded by the irreducible noise σ^2