STEVENS INSTITUTE OF TECHNOLOGY

Machine Learning Fundamentals: Bias vs. Variance

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Bias vs. Variance

- Whenever we discuss model prediction, its important to understand prediction errors (bias and variance).
- There is a tradeoff between a models ability to minimize bias and variance.
- Gaining a proper understanding of these errors would help us not only to build accurate models but also to avoid the mistake of **overfitting** and **underfitting**.
- **Bias:** Bias is the difference between the average prediction of our model and the correct value which we are trying to predict.
- **Variance:** Variance is the variability of model prediction for a given data point or a value which tells us spread of our data.

Bias vs. Variance

- **Bias:** Bias is the difference between the average prediction of our model and the correct value which we are trying to predict.
  - Model with high bias pays very little attention to the training data and oversimplifies the model.
  - It always leads to high error on training and test data.
- **Variance:** Variance is the variability of model prediction for a given data point or a value which tells us spread of our data.
  - Model with high variance pays a lot of attention to training data and does not generalize on the data which it hasnt seen before.
  - As a result, such models perform very well on training data but has high error rates on test data.

Bias vs. Variance : Mathematically

- Let the variable we are trying to predict as Y and other covariates as X. We assume there is a relationship between the two such that

$$Y = f(X) + e$$

  Where e is the error term and its normally distributed with a mean of 0.

- We will make a model $\hat{f}(X)$ of $f(X)$ using linear regression or any other modeling technique. So the expected squared error at a point x is

$$Err(x) = E\left[\left(Y - \hat{f}(x)\right)^2\right]$$

  where $E[\cdot]$ is the expectation.

- As $Y = f(x) + e$, the $Err(x)$ can be further decomposed as

$$Err(x) = E\left[\left(f(x) + e - \hat{f}(x)\right)^2\right] = E\left[\left(f(x) - \hat{f}(x)\right)^2 + e^2 + 2e[f(x) - \hat{f}(x)]\right]$$

Bias vs. Variance : Mathematically

- The $Err(x)$ can be further decomposed as

$$\begin{aligned} Err(x) =& E\left[\left(f(x)-\hat{f}(x)\right)^2 + 2e[f(x)-\hat{f}(x)] + e^2\right] \\ =& E\left[\left(f(x)-\hat{f}(x)\right)^2 + 2e[f(x)-\hat{f}(x)]\right] + \sigma_e^2 \end{aligned}$$

where $E[e^2] = \sigma_e^2$.

- The noise term e is independent of $f(x)$ and $\hat{f}(x)$, then the expectation $E\left[2e\left(f(x)-\hat{f}(x)\right)\right] = 0$.

$$\begin{aligned} Err(x) =& E\left[\left(f(x)-\hat{f}(x)\right)^2 + 2e[f(x)-\hat{f}(x)]\right] + \sigma_e^2 \\ =& E\left[\left(f(x)-\hat{f}(x)\right)^2\right] + 0 + \sigma_e^2 \end{aligned}$$

Bias vs. Variance : Mathematically

- Reform the term $E[(f(x) - \hat{f}(x))^2]$

$$
\begin{aligned}
& E\left[\left(f(x) - \hat{f}(x)\right)^2\right] \\
=& E\left[\left(\hat{f}(x) - f(x)\right)^2\right] \\
=& E\left[\left(\underbrace{\hat{f}(x) - E[\hat{f}(x)]} + \underbrace{E[\hat{f}(x)] - f(x)}\right)^2\right] \\
=& E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \left(E[\hat{f}(x)] - f(x)\right)^2 + 2E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)\left(E[\hat{f}(x)] - f(x)\right)\right] \\
=& \text{Variance} + \text{Bias}^2 + 2E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)\left(E[\hat{f}(x)] - f(x)\right)\right]
\end{aligned}
$$

where Variance $= E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right]$ and Bias $= E[\hat{f}(x)] - f(x)$.

- Note in the above equation, the bias ($E[\hat{f}(x)]$ - $f(x)$) is a deterministic term and the expectation operation vanished over the bias.

Bias vs. Variance : Mathematically

- We further simplify the term,

$$
\begin{aligned}
&E\left[\left(f(x)-\hat{f}(x)\right)^2\right] \\
=&\text{Variance}+\text{Bias}^2+2E\left[\left(\hat{f}(x)-E[\hat{f}(x)]\right)\left(E[\hat{f}(x)]-f(x)\right)\right]
\end{aligned}
$$

0

- As aforementioned, the bias term ($E[\hat{f}(x)]$ - $f(x)$) is independent of the expectation operator, we can move it out of the expectation,

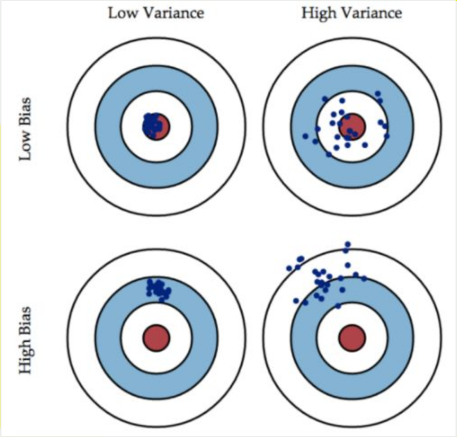
$$
\begin{aligned}
&E\left[\left(\hat{f}(x)-E[\hat{f}(x)]\right)\left(E[\hat{f}(x)]-f(x)\right)\right] \\
=&E\left[\left(\hat{f}(x)-E[\hat{f}(x)]\right)\right]\cdot\left(E[\hat{f}(x)]-f(x)\right) \\
=&\left(E[\hat{f}(x)]-E[\hat{f}(x)]\right)\cdot\left(E[\hat{f}(x)]-f(x)\right)=0
\end{aligned}
$$

- Overall we have the error term

$$
Err(x)=E\left[\left(f(x)-\hat{f}(x)\right)^2\right]+\sigma_e^2=\text{Variance}+\text{Bias}^2+\sigma_e^2
$$

Bias vs. Variance : Tradeoff

- In the error term, the noise variance σ_e^2 is irreducible and therefore we can only work on the bias and variance terms.



Underfitting vs. Overfitting

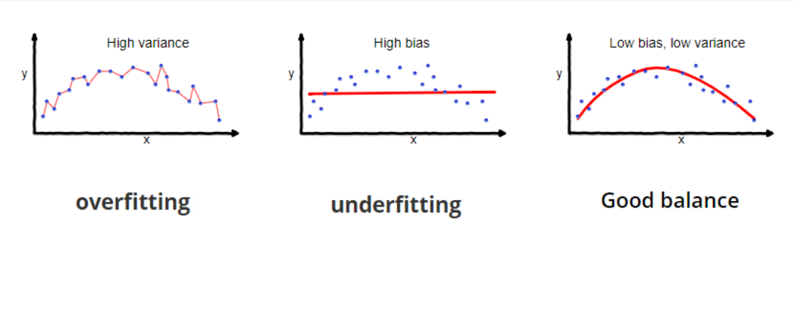
- In supervised learning, **underfitting** happens when a model unable to capture the underlying pattern of the data.
- These models usually have high bias and low variance.
- It happens when we have very less amount of data to build an accurate model or when we try to build a linear model with a nonlinear data.
- For instance, these kind of models are very simple to capture the complex patterns in data like Linear and logistic regression.

Underfitting vs. Overfitting

- In supervised learning, **overfitting** happens when our model captures the noise along with the underlying pattern in data.
- It happens when we train our model a lot over noisy dataset.
- These models have low bias and high variance. These models are very complex like Decision trees which are prone to overfitting.

Underfitting vs. Overfitting

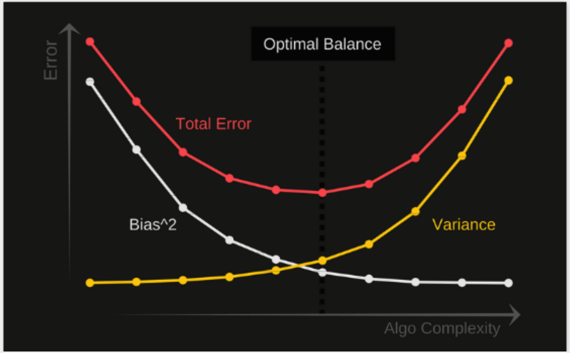
- If our model is too simple and has very few parameters then it may have high bias and low variance.
- On the other hand if our model has large number of parameters then its going to have high variance and low bias.
- So we need to find the right/good balance without overfitting and underfitting the data. This tradeoff in complexity is why there is a tradeoff between bias and variance.



Bias vs. Variance: Tradeoff

- To build a good model, we need to find a good balance between bias and variance such that it minimizes the total error.

$$\text{Total Error} = \text{Bias}^2 + \text{Variance} + \text{Noise}$$



Underfitting vs. Overfitting

- Let us assume we have both training and testing data sets.
- Let us assume in a classification example, the best model, i.e., the benchmark model, whatever using human or machine, can reach 0% error rate.
- If the model learned on training data has an error rate $\gg 0\%$, for instance, 15%, then there is a big bias, i.e., underfitting.
- If the learned model applies for the testing data has an error rate 30%, then there is a big variance at this model.
- Comparing both training and testing data error rates with the benchmark model, this learning method has both big bias and big variance.
- If the same model applies for the testing data has an error rate 16%, then there is a big bias but small variance at this model.

Underfitting vs. Overfitting

- Let us assume we have both training and testing data sets.
- Let us assume in a classification example, the best model, i.e., the benchmark model, whatever using human or machine, can reach 0% error rate.

Training Error Rate	Testing Error Rate	Bias vs. Variance	Note
15 %	30 %	big bias, big variance	Underfitting
15 %	16 %	big bias, small variance	Underfitting
1 %	15%	small bias, big variance	Overfitting
1%	2%	small bias, small variance	